

Richard Kawabe Tauscher

Vorstellung & Projekte

Inhalt

- Kenntnisse und Kompetenzen

Kenntnisse und Kompetenzen



BATTERIETECH. & LIB-PRODUKTION

Zellfertigung

Slurryherstellung & Coating

Zellenbau

Charakterisierung & Tests

Raten-Tests, mechano-physikalische und elektrochemische Methoden

Modellierung & Simulation

Alterungsmechanismen, Diffusionsmodelle, Kinetik, elektrochemische Parameteranalyse



PROGRAMMIERUNG & SIMULATION

Programmiersprachen (e-CF Level)

(2-3) MATLAB

(2) C++, Python

(1) HTML, XML, C#, VB

Modellierung & Simulation

1-D Modellierung, KMC Simulation, numerische Methoden, Datenanalyse

BMW-Industriepraktikum | Ziel/Aufgaben

Zielsetzung

- Untersuchung von durch Fremdfirmen hergestellter Elektroden
 - Gleiche chemische Zusammensetzung
 - Verschiedene Herstellungsprozesse
- Qualitätsbeurteilung durch schnelle und einfache Methoden

Aufgabe

- Methodenscreening geeigneter Prüfmethoden
- Korrelation mechano-physikalischer und elektrochemischer Eigenschaften

Aufgabengebiet

- Recherche von Prüfmethoden
- Kontaktherstellung zu Messfirmen
- Beauftragung von Fremdfirmen zu Materialprüfungen
- Probenpräparation
- Messmethode erstellen und verbessern
- Messungen an Proben
- Bau von funktionierenden Halb- und Vollzellen
- Auswertung von Messergebnissen

BMW-Industriepraktikum | Verfahren

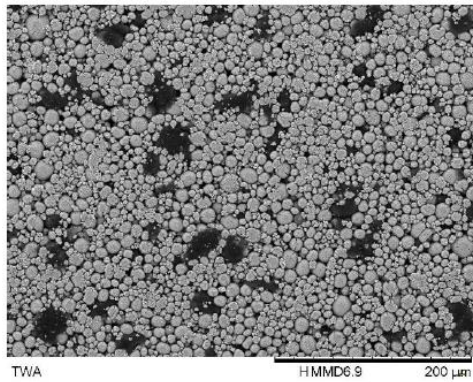
Angewandte Verfahren

- Stirnzugprüfung
- Dornbiegeprüfung
- Massenverlustmessung
- Widerstandsmessung
- REM
- QCSM-Härteprüfung
- Durchstoß- / Berstprüfung
- Kontaktwinkelmessung
- 3D-Oberflächenscanning (FRT-Rauhigkeitsmessung)
- Elektrochemische Ratentests

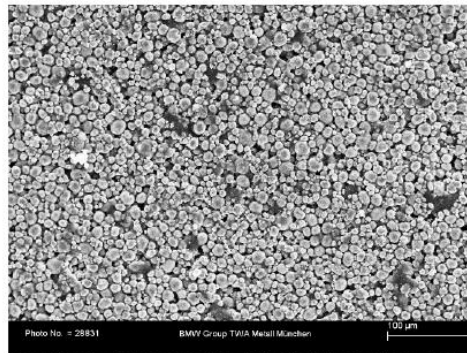
BMW-Industriepraktikum | Ergebnisse

04.2.3 REM Aufnahmen

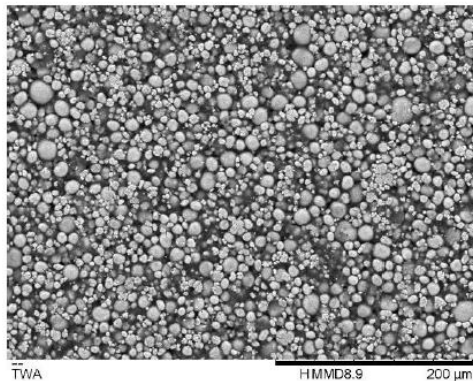
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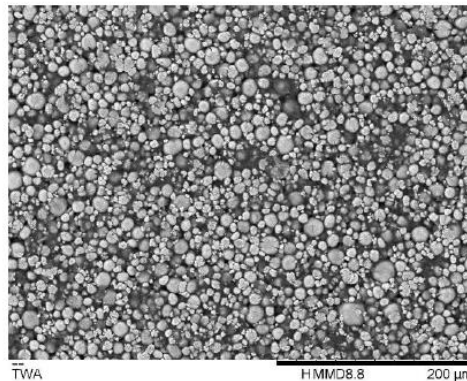
H3



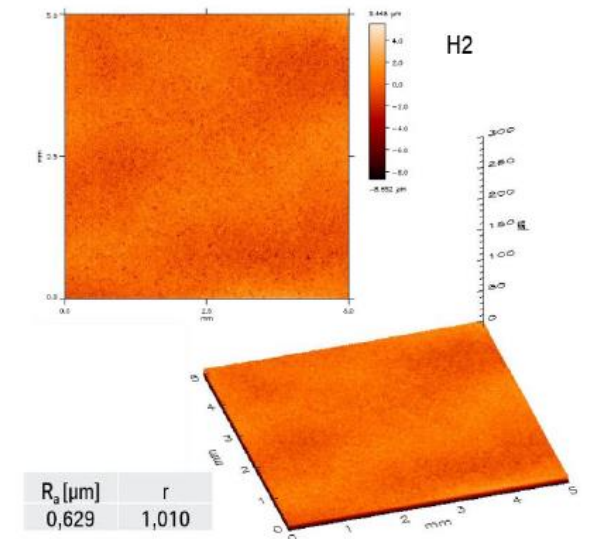
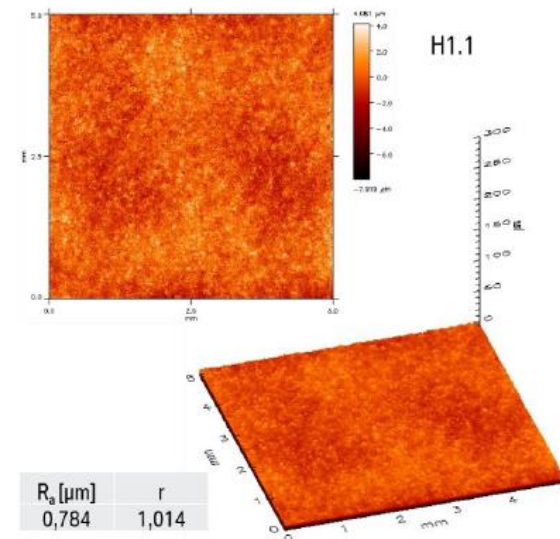
H1.2



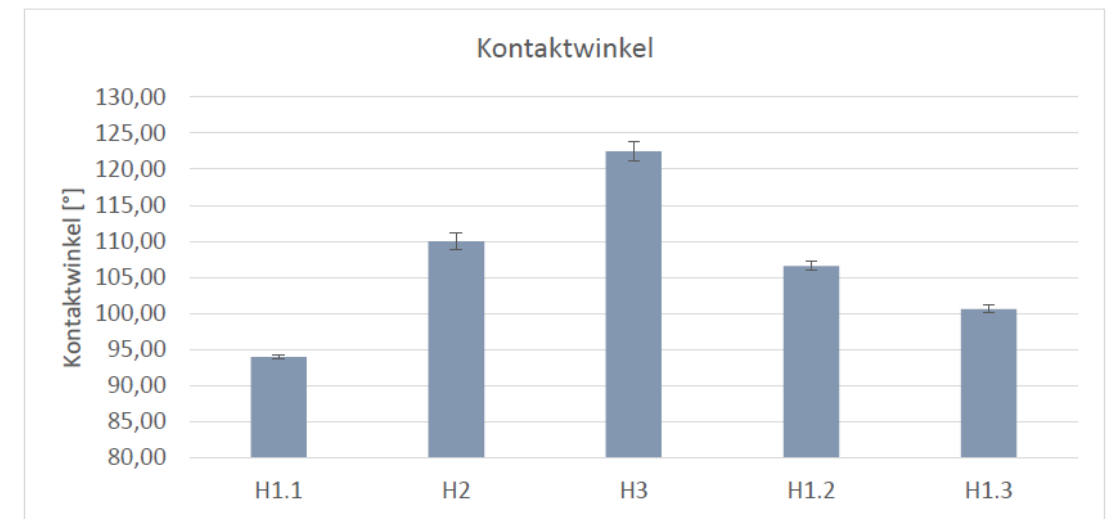
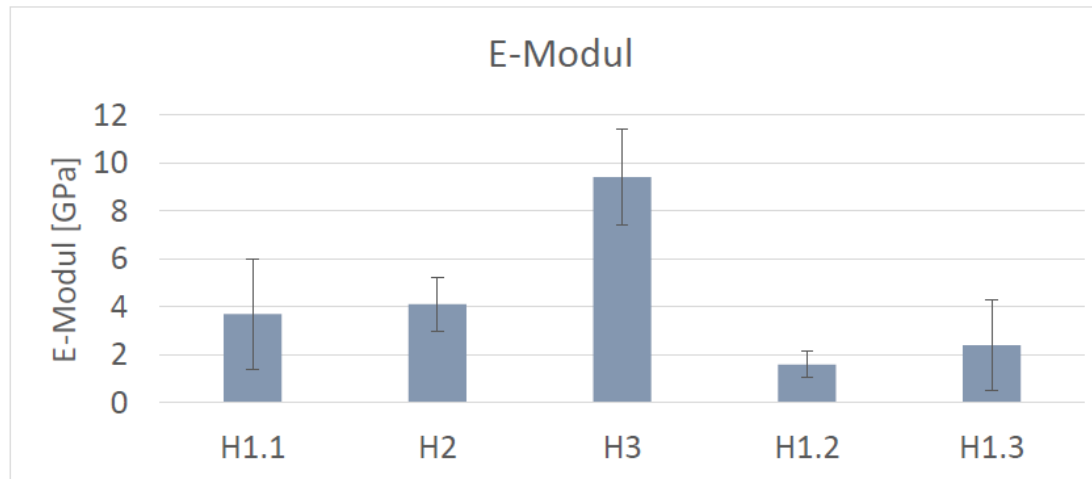
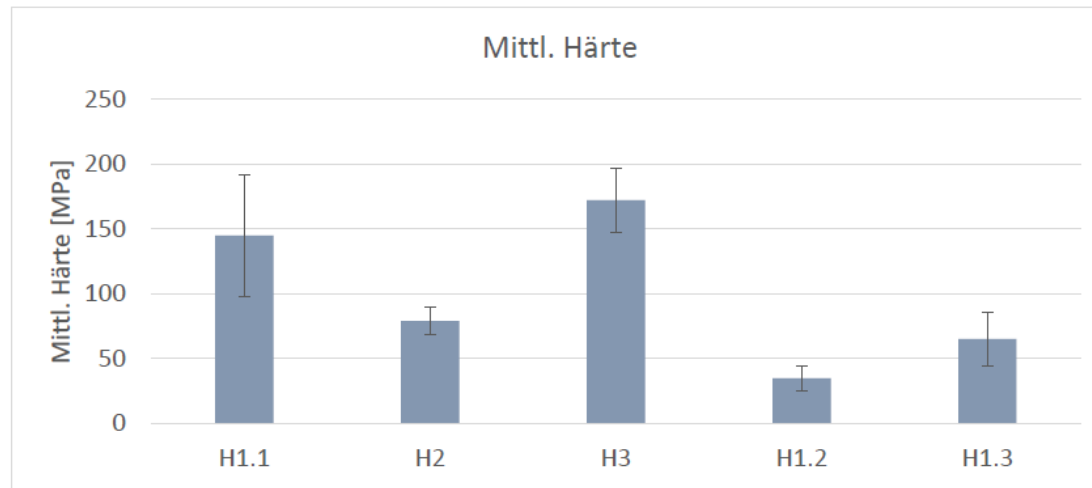
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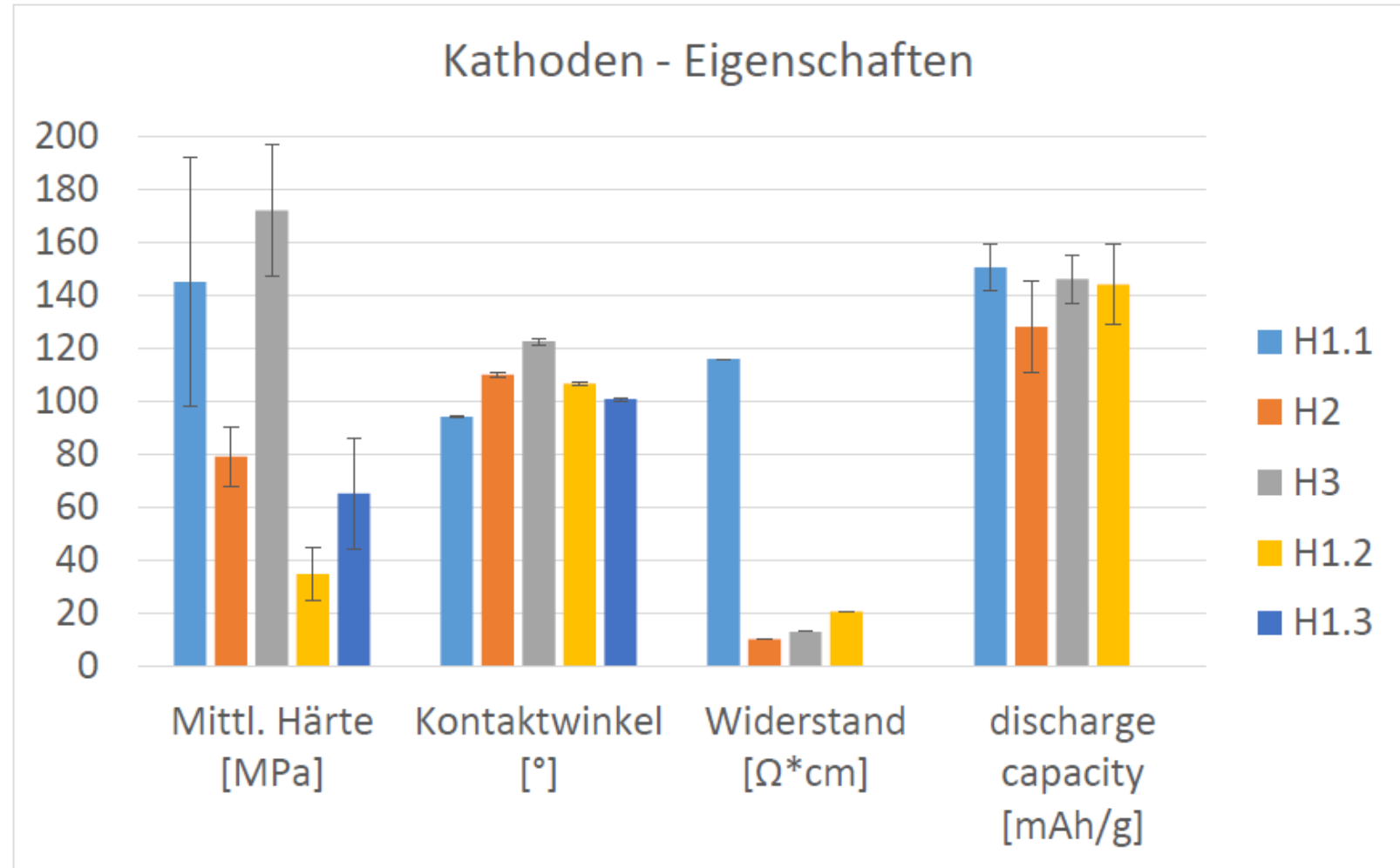
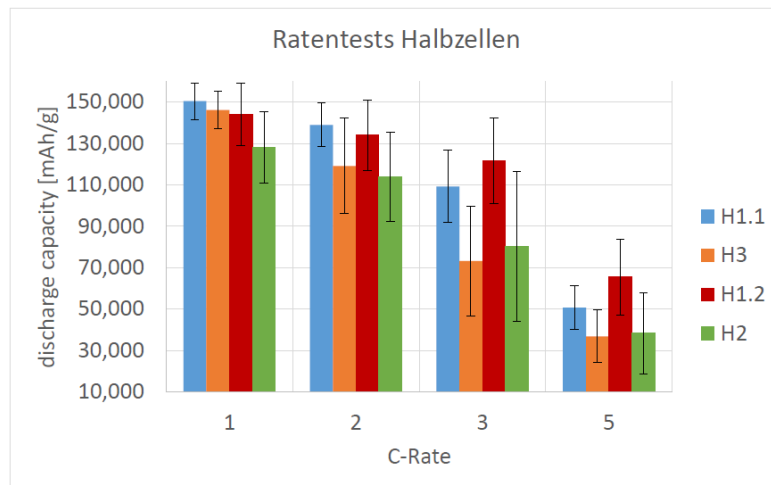
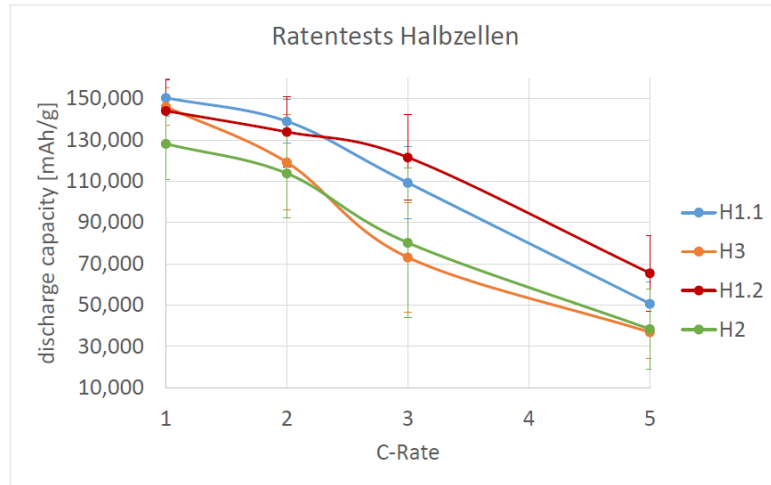
FRT – 3D-Oberflächenscan



BMW-Industriepraktikum | Ergebnisse



BMW-Industriepraktikum | Ergebnisse



BA Fraunhofer IPA | Ziel/Aufgaben

Zielsetzung

- Konzeption und Aufbau einer Anlage zur kontinuierlichen Pastenherstellung
 - Automatisierung und Digitalisierung
 - Inline-Charakterisierung des Produktes
- Untersuchung der Prozessparameter
 - Korrelation zwischen Prozessparameter und Pastenqualität

Aufgabe

- Konzeption und Aufbau der Anlage
- Optimierung und Fehlerbehebung
- Testreihen mit statistischer Versuchsplanung (DoE)

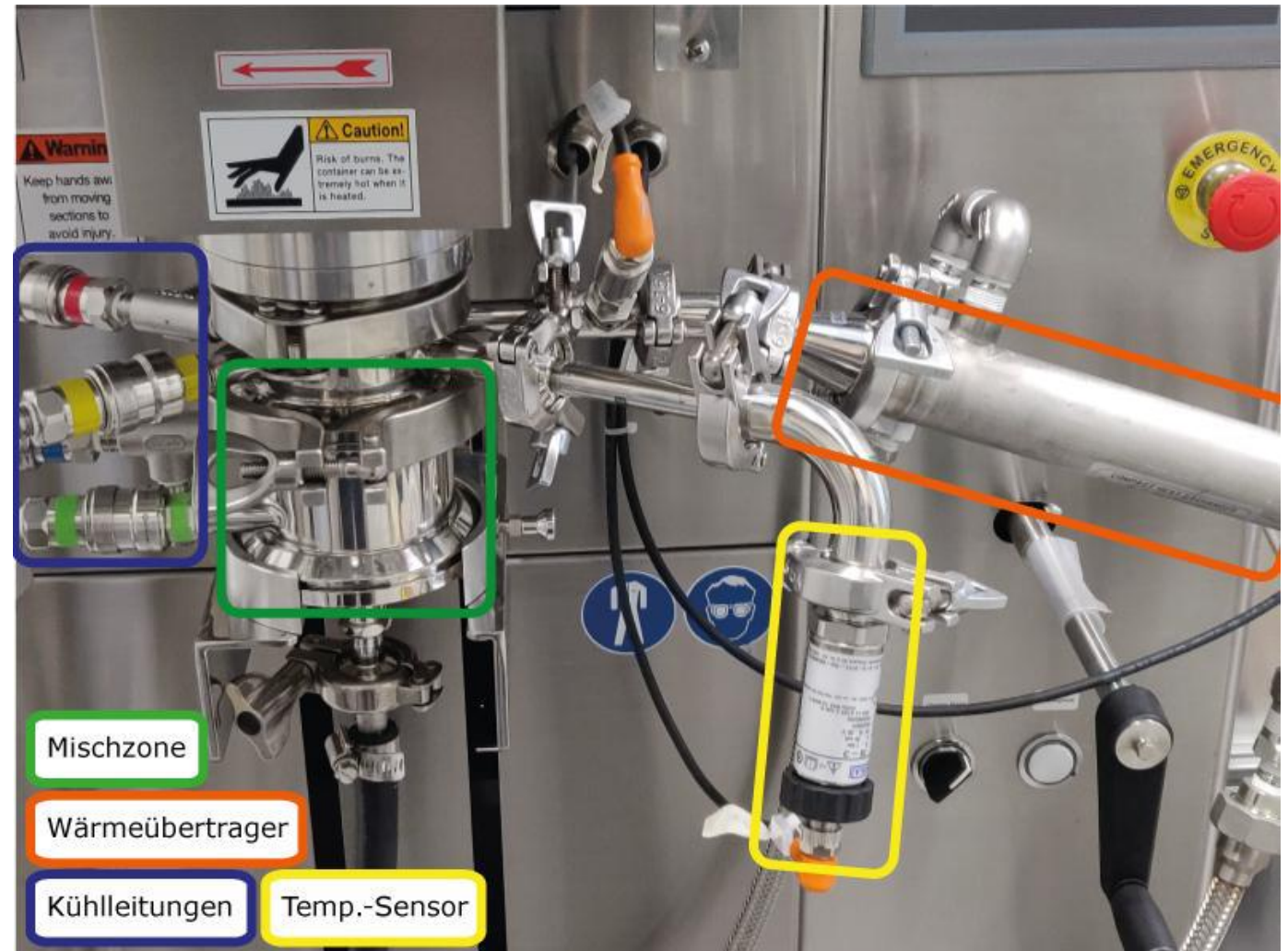
Aufgabengebiet

- Berechnungen zu Strömen und Drücken
- Aufbau der Anlage
- Unterstützung der Gefährdungsbeurteilungen
- Überprüfung Sensoren/Schutzeinrichtungen
- Erstellung von Betriebsanweisungen
- Beschaffung von Ausrüstung (inkl. PSA)
- Kalibrierung Messgeräte
- Validierung Messungen
- Versuchsdurchführung mit DoE
- Konzeption digitale Produktionstelle

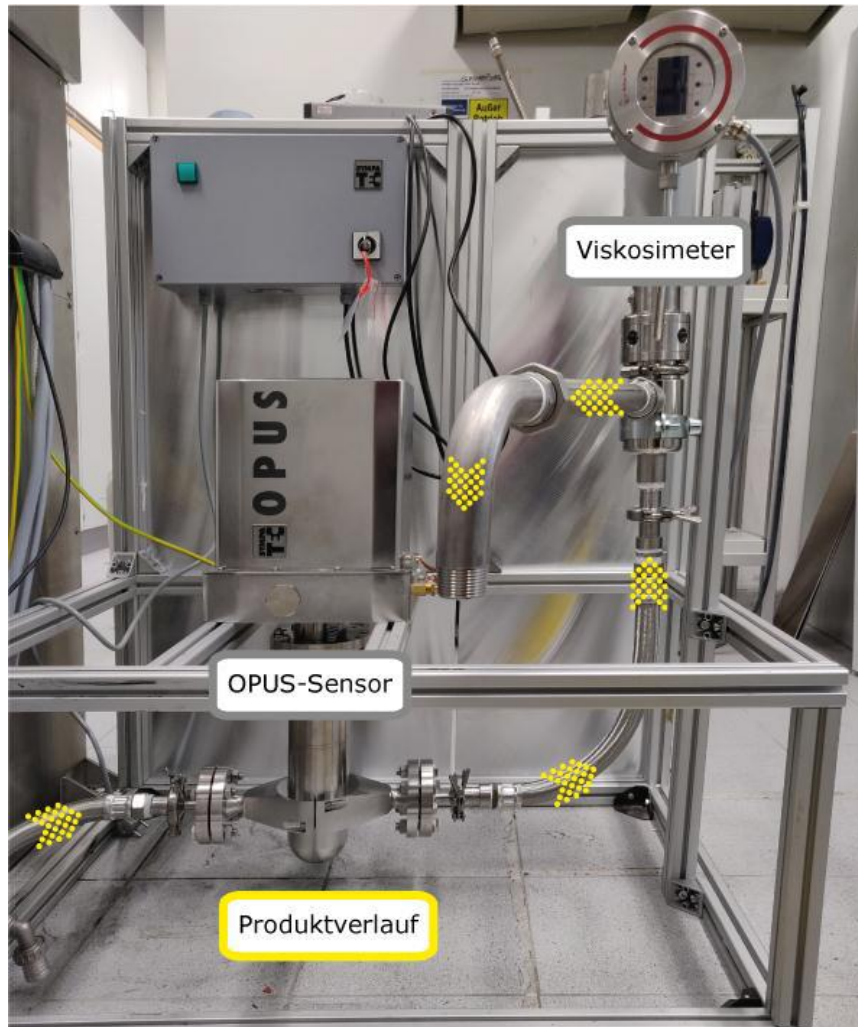
BA Fraunhofer IPA | Aufbau



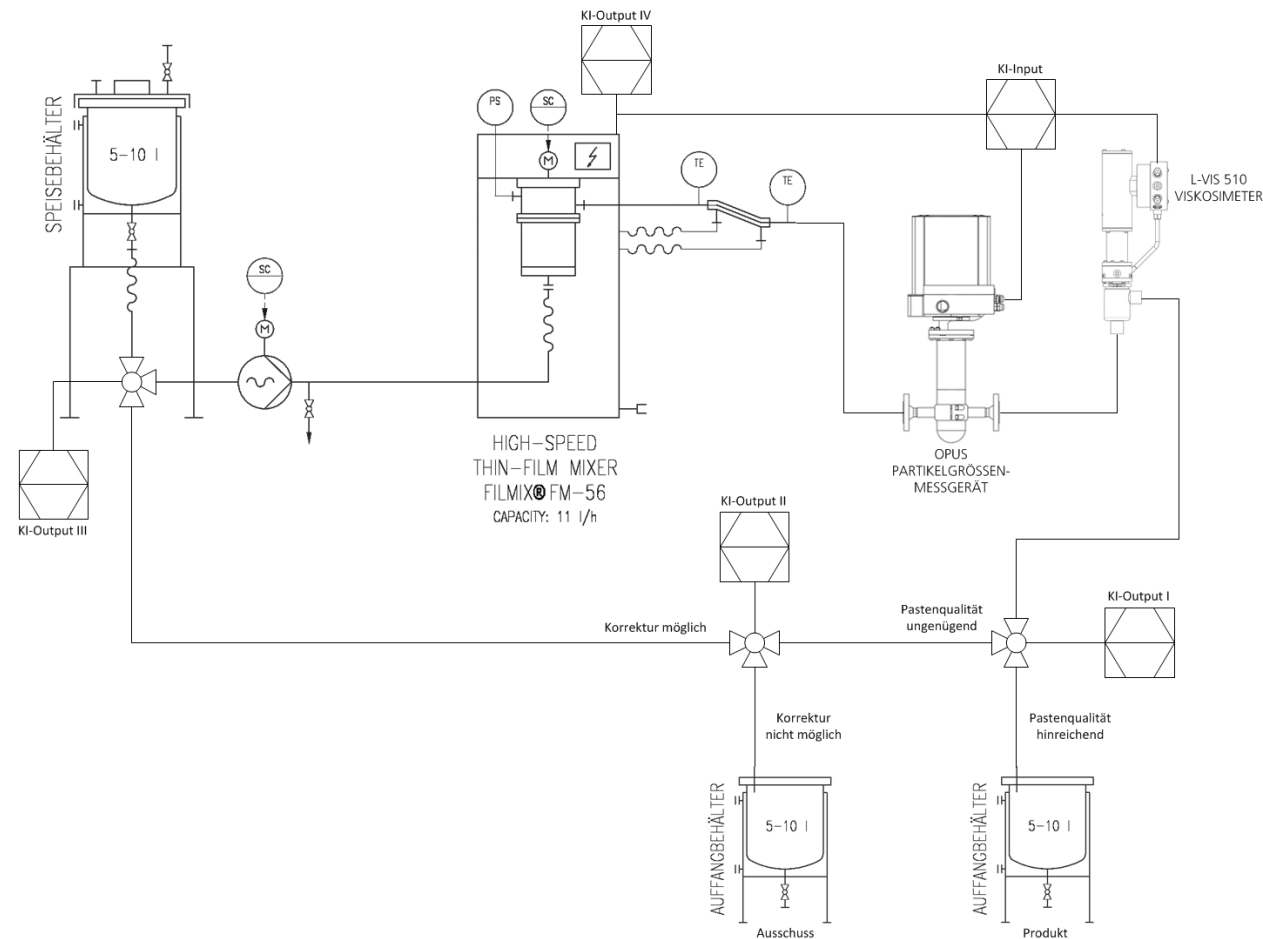
BA Fraunhofer IPA | Aufbau



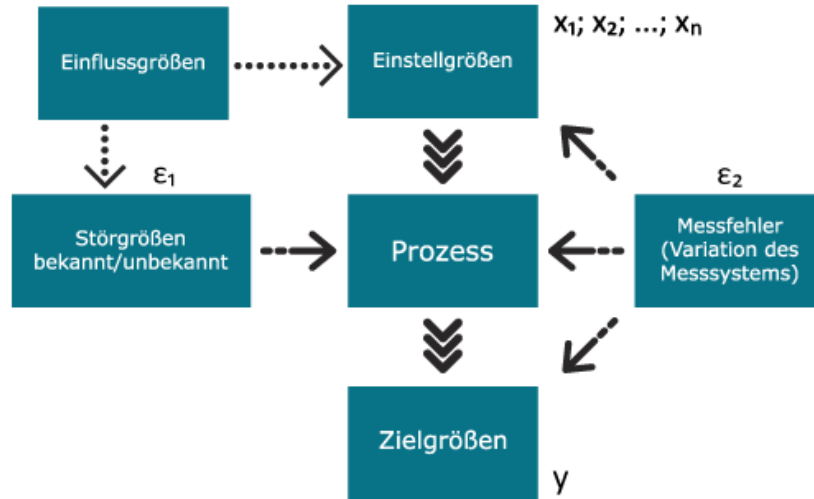
BA Fraunhofer IPA | Aufbau



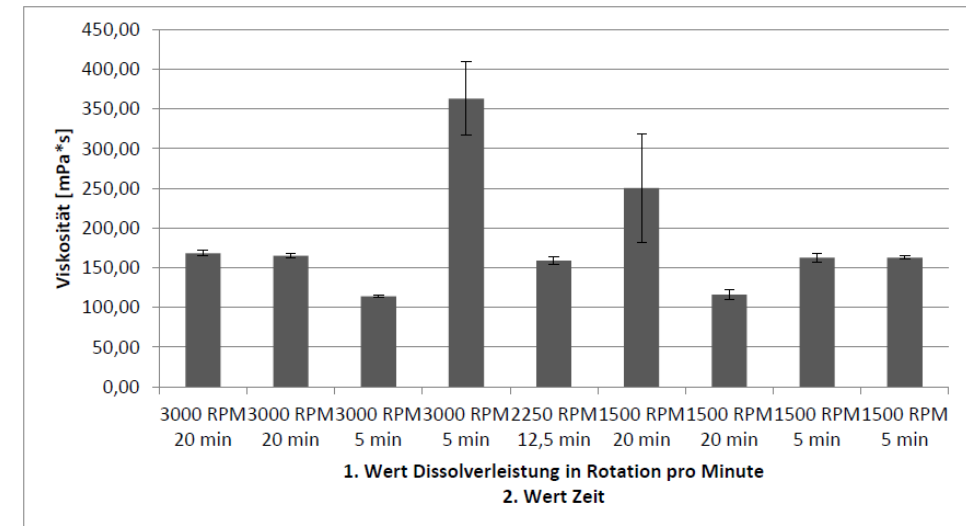
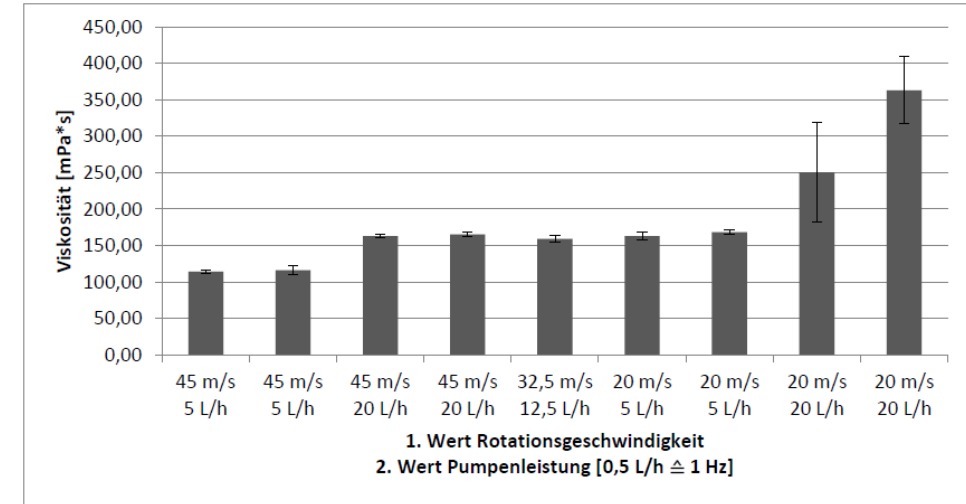
BA Fraunhofer IPA | Produktionszelle



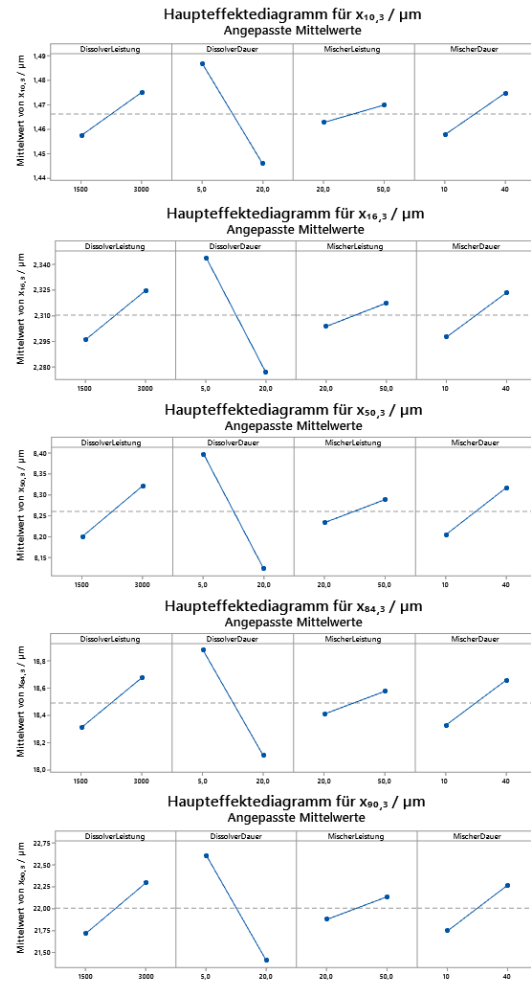
BA Fraunhofer IPA | DoE



RunOrder	Dissolver		Filmix	
	Leistung	Dauer	Rotorgeschw.	Verweildauer
	[rpm]	[min]	[m/s]	[Hz]
1	3000	5	45	10
2	1500	5	20	10
3	1500	20	20	40
4	1500	20	45	10
5	3000	20	20	10
6	2250	12,5	32,5	25
7	1500	5	45	40
8	3000	5	20	40
9	3000	20	45	40



BA Fraunhofer IPA | Ergebnisse



MA KIT: IAM-ET | Ziel/Aufgaben

Zielsetzung

- Elektrochemische Modellierung der SEI Degradation bei thermischer Alterung

Aufgabe

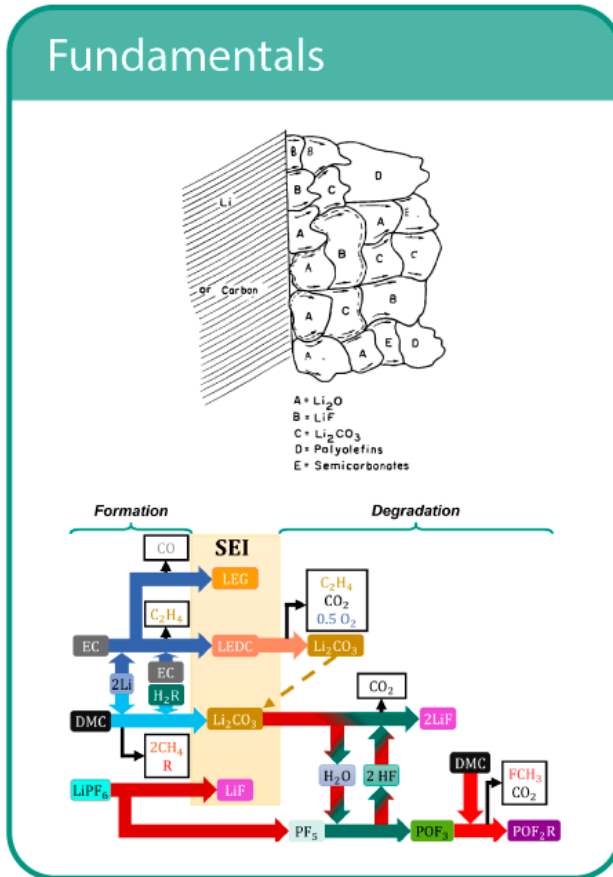
- Simulation einer Batteriezelle
- Modelle für SEI Abbildung und ablaufende chemisch-physikalische Prozesse
- Implementierung eines Reaktionsnetzwerks
- Parametereinstellung mithilfe OEMS-Prüfstand

Aufgabengebiet

- Theorie für Modellierung von Batteriesystemen
- Programmierung von
 - Simulationsbereich
 - Temperaturverläufe
 - SoC-Initiierung
 - Diffusion
 - Volumensänderung
- Datenanalyse und -Abgleich

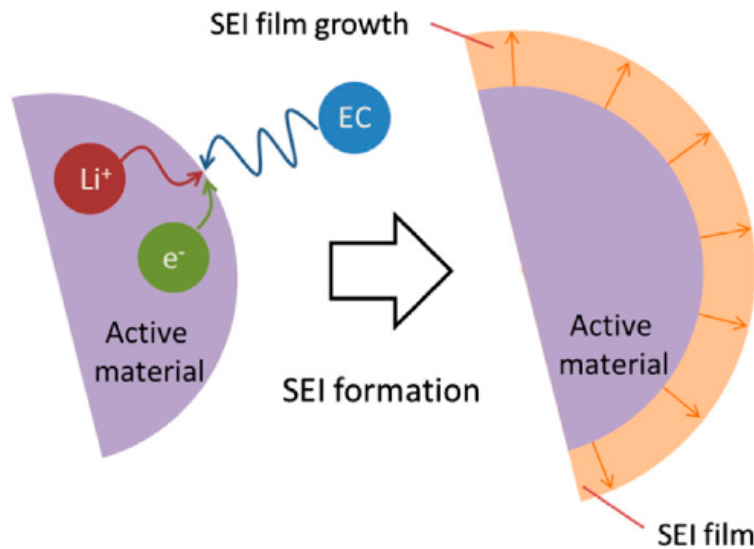
Contents

Fundamentals



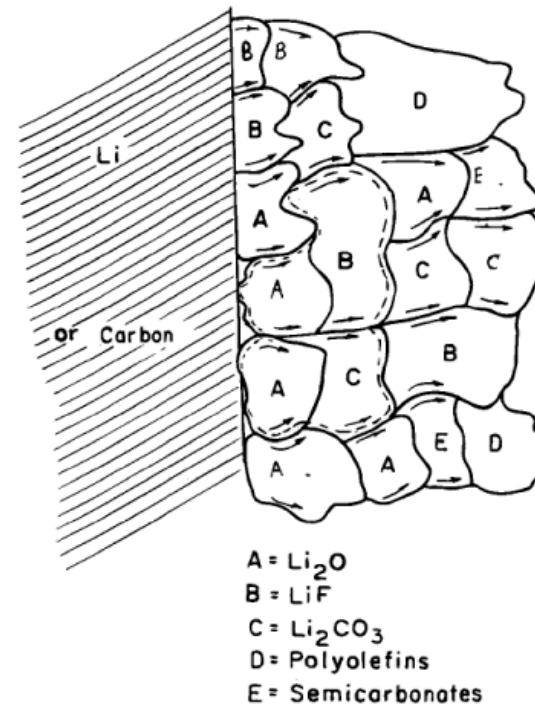
Fundamentals - SEI

Solid Electrolyte Interphase - Formation



- SEI Formation during cycling
- Composition depends on materials

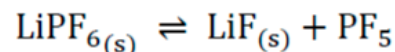
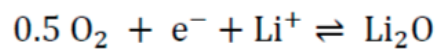
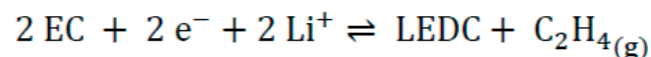
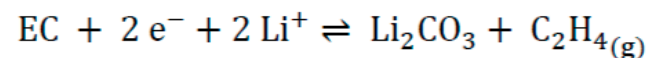
SEI Species and Properties



- Inner anorganic layer
 - Li_2O
 - LiF
 - Li_2CO_3
- Outer organic layer
 - LEDC
 - Li_2CO_3
- Higher porosity on outer layer
- Isolating properties
- SEI has stabilizing properties

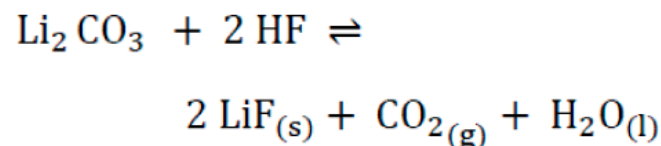
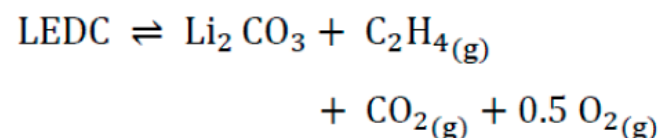
Fundamentals - Reactions

SEI Formation Reactions



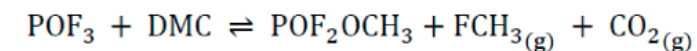
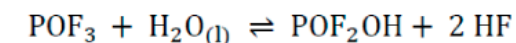
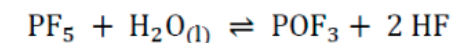
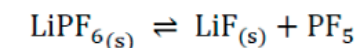
- Mostly reactions with Lithium
- Mainly on first cycling

SEI Degradation Reactions



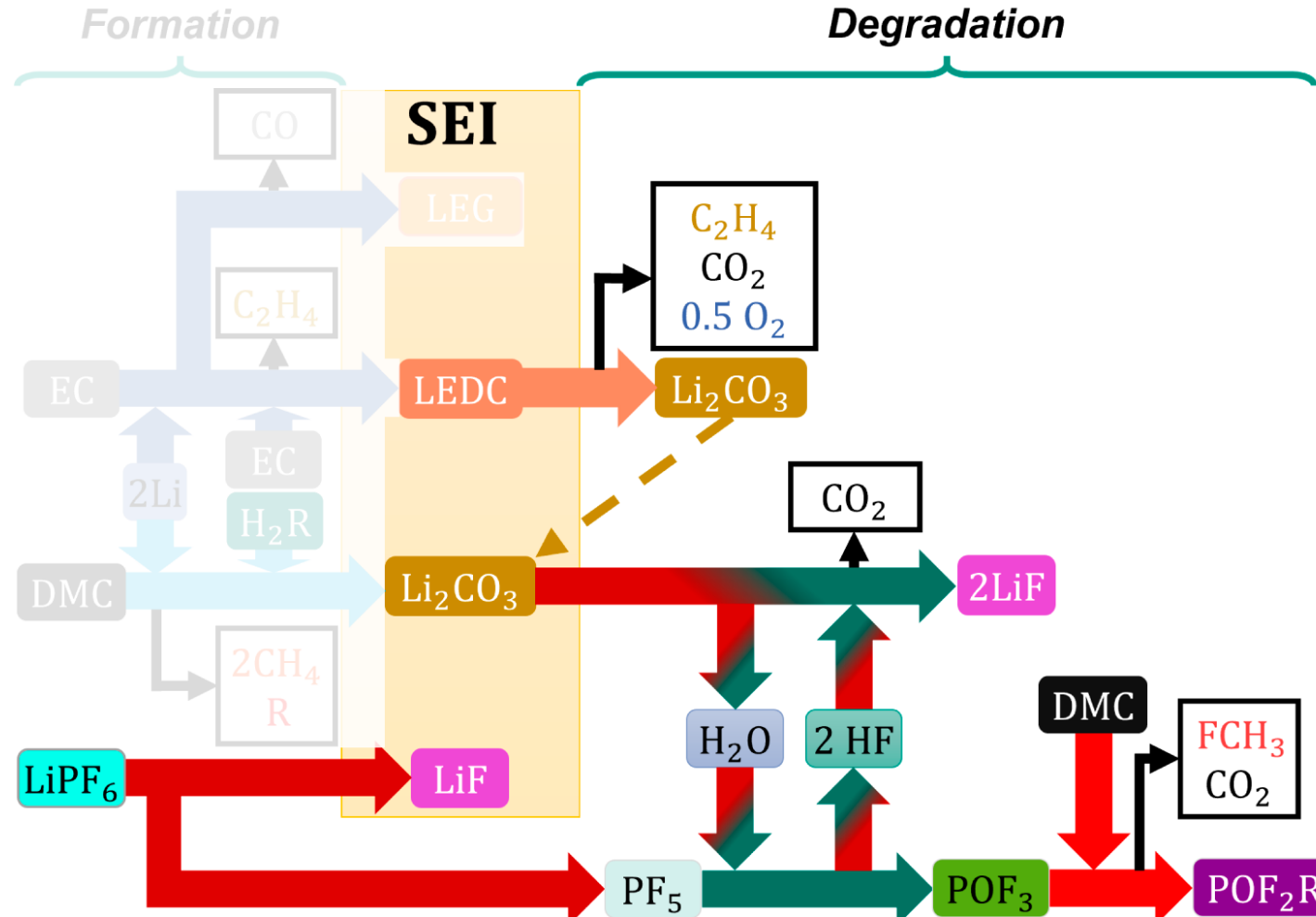
- High gaseous species output
- Hydrofluoric acid can lead to high degradation

Salt Decomposition Reactions

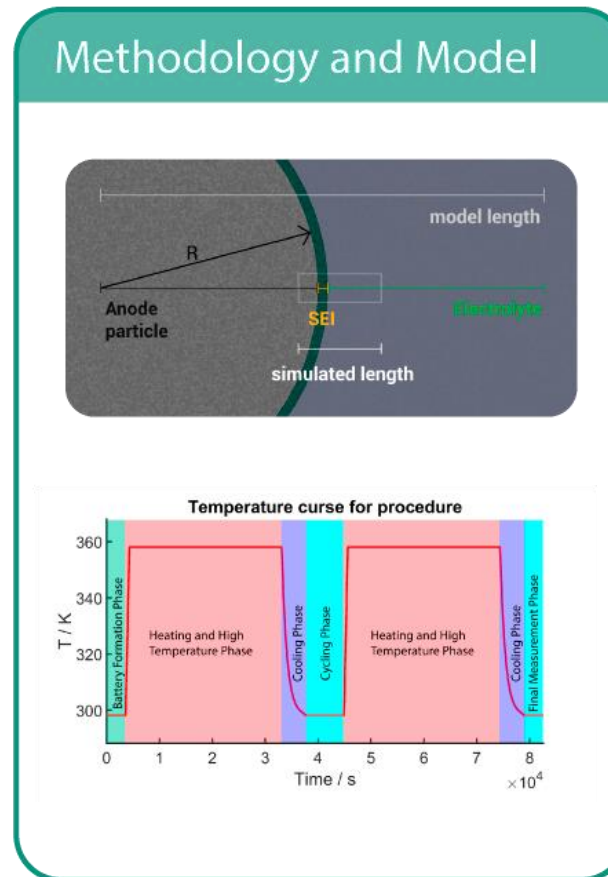


- Contamination of cell with water leads to hydrofluoric acid production
- Formation of phosphorus oxyfluoride derivatives

(Electro-)Chemical Reactions



Contents



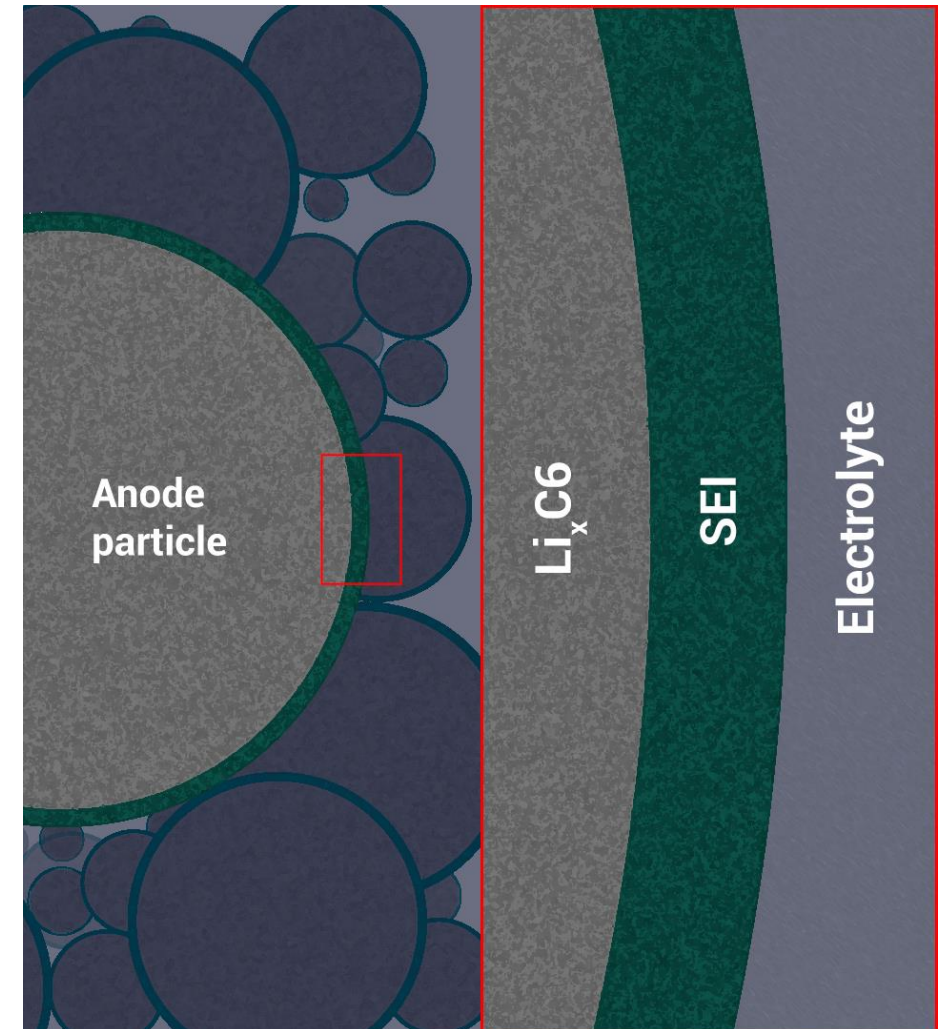
Simulation Structure

Simulation Basis: Experimental Setup

- OEMS (on-line electrochemical mass spectrometry)
- Measurement procedure with heating process

Model basis: Single Particle Model

- Electrode represented by single particle
- Chemical reactions accounting for solid SEI species, electrolyte and gases
- Mass transport via diffusion



Characteristics – Model and Simulation Area

Model Parameters

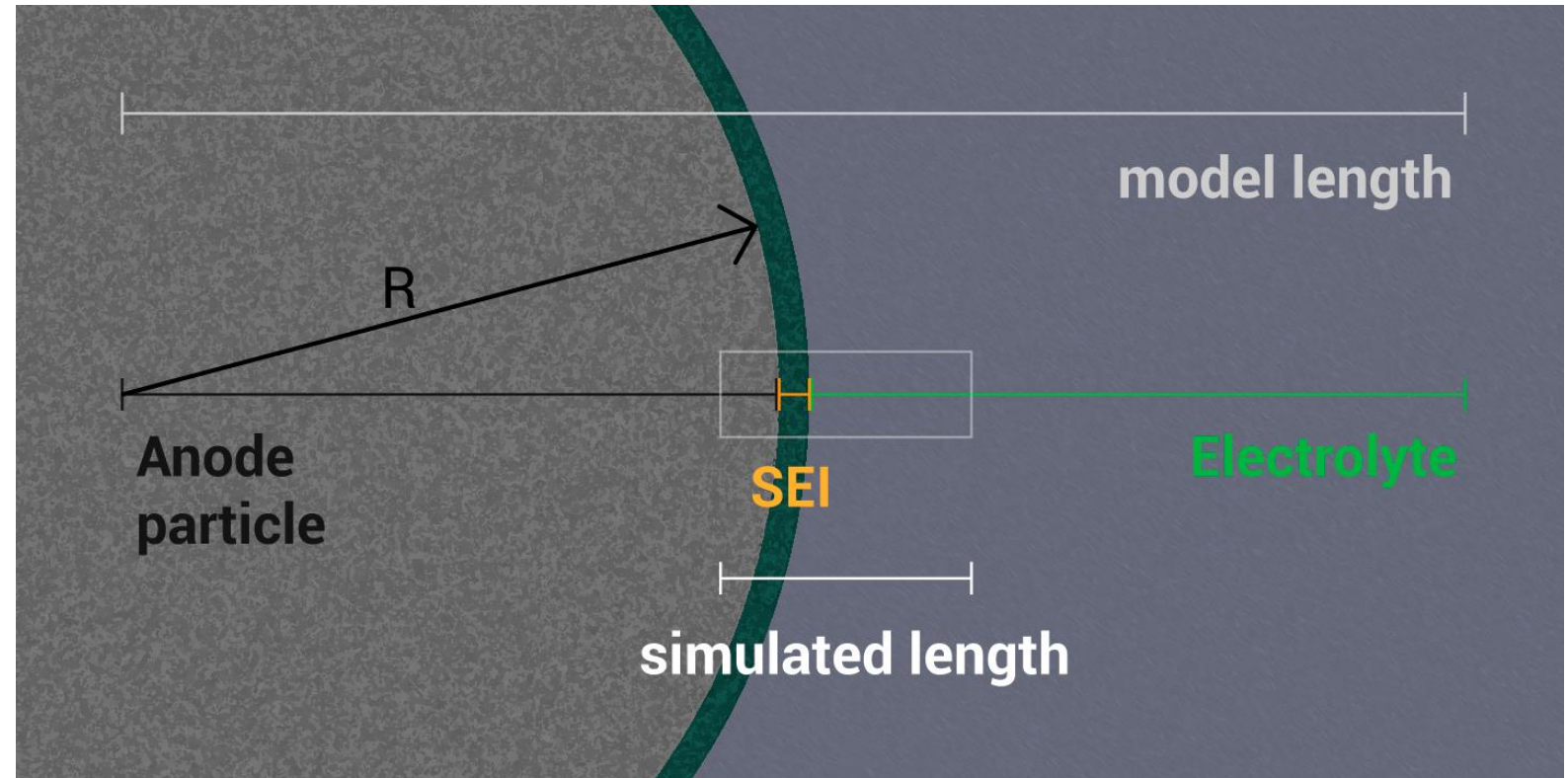
Model length defined by:

- Equal length anode and electrolyte
- SEI thickness

Simulation Characteristics

Simulation length

- Computational restrictions
- Shorter than model length
- SEI fully simulated



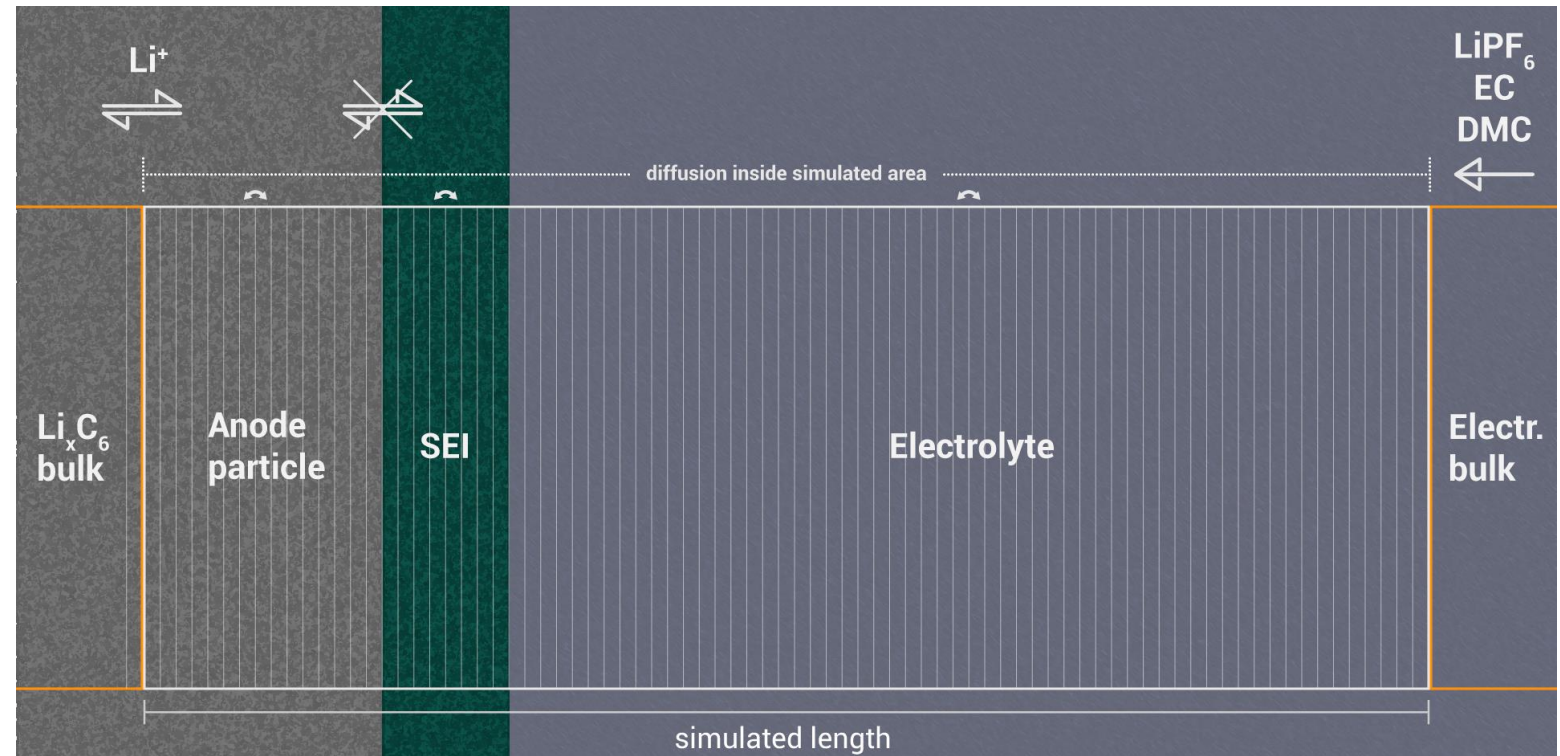
Characteristics – Diffusion Model

Diffusion - Fick's 2nd law

$$\frac{\partial c_a}{\partial t} = D_a \frac{\partial^2 c_a}{\partial x^2}$$

Model Assumptions

- Three main areas
- Defined volume elements (VE)
- Diffusion between VEs
- Diffusion restricted between anode and SEI area
- Outside sim area: bulk
- Diff. only by fluid species



Parameters for Species

Initial Concentration

SEI species

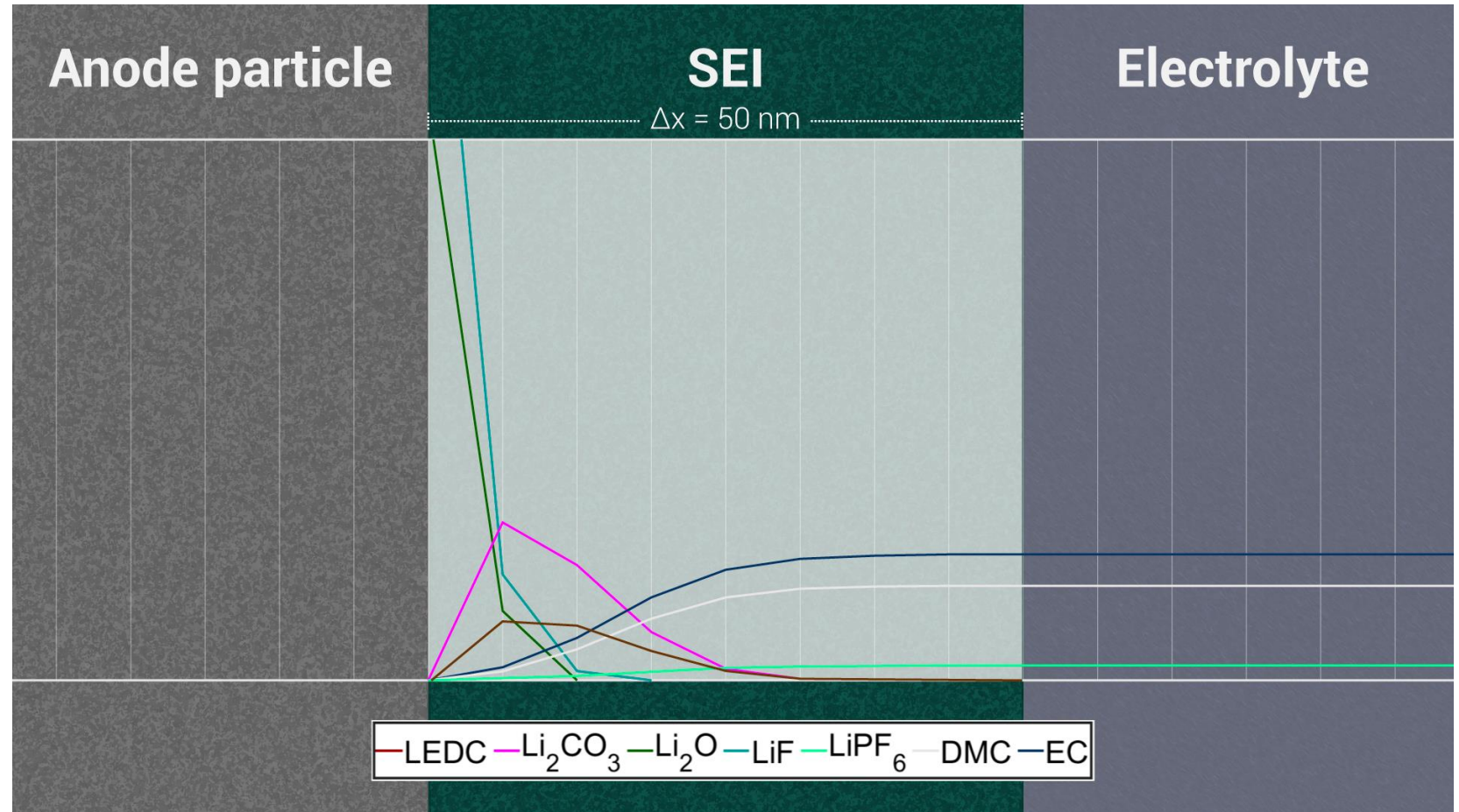
- Bisection method
- $x = 0$ nm
 - 0% porosity
 - 100% LiF/Li₂O
 - 0% LEDC
- $x = 50$ nm
 - 100% porosity
 - 0% LiF/Li₂O
 - 100% LEDC
- Li₂CO₃ max. volume in between

Electrolyte

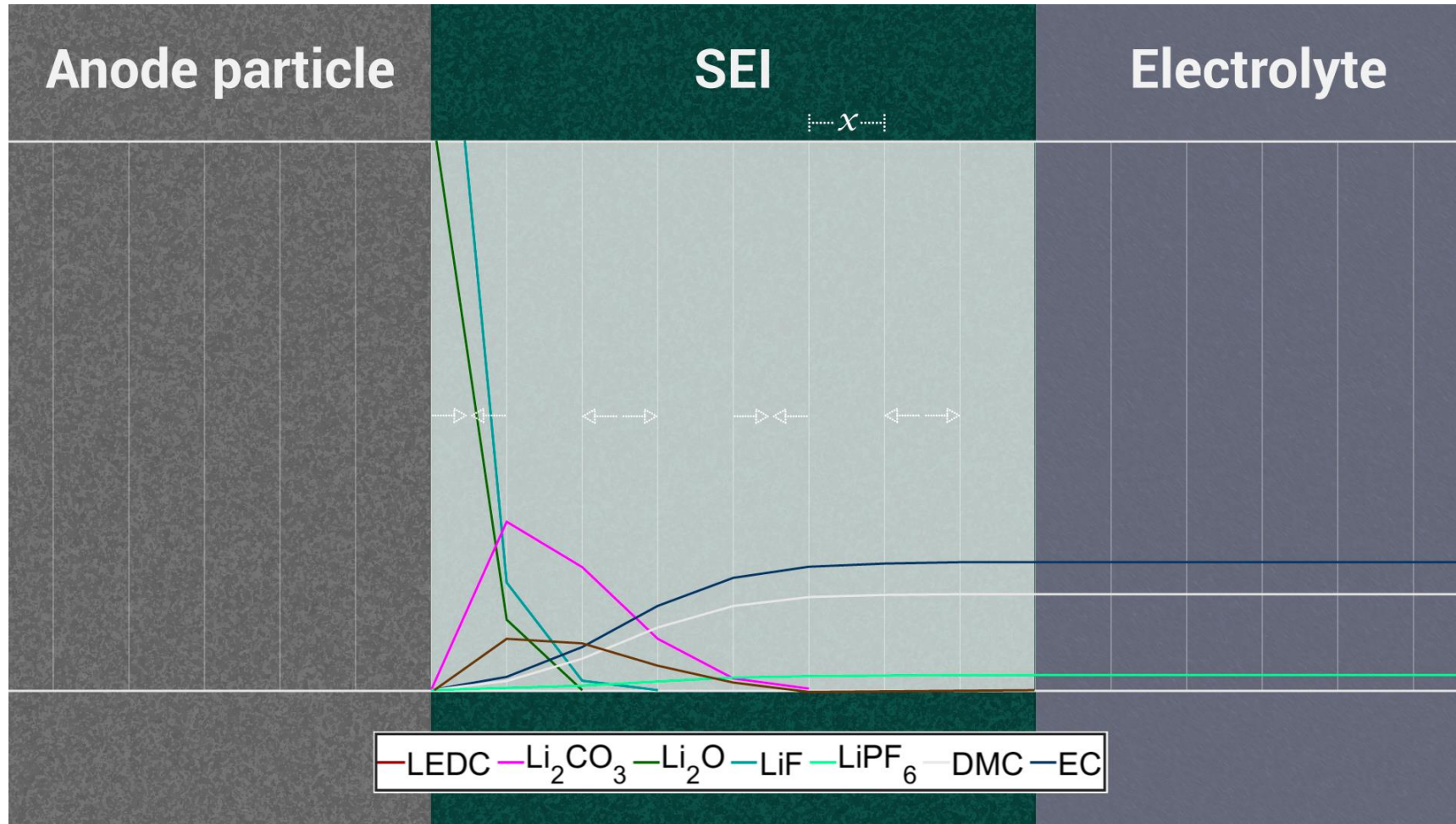
- 1:1 EC/DMC
- 1M LiPF₆
- 50 ppm H₂O

Anode particle

- Total volume Li_xC₆



Characteristics – Dynamic Volume Model



Model assumption

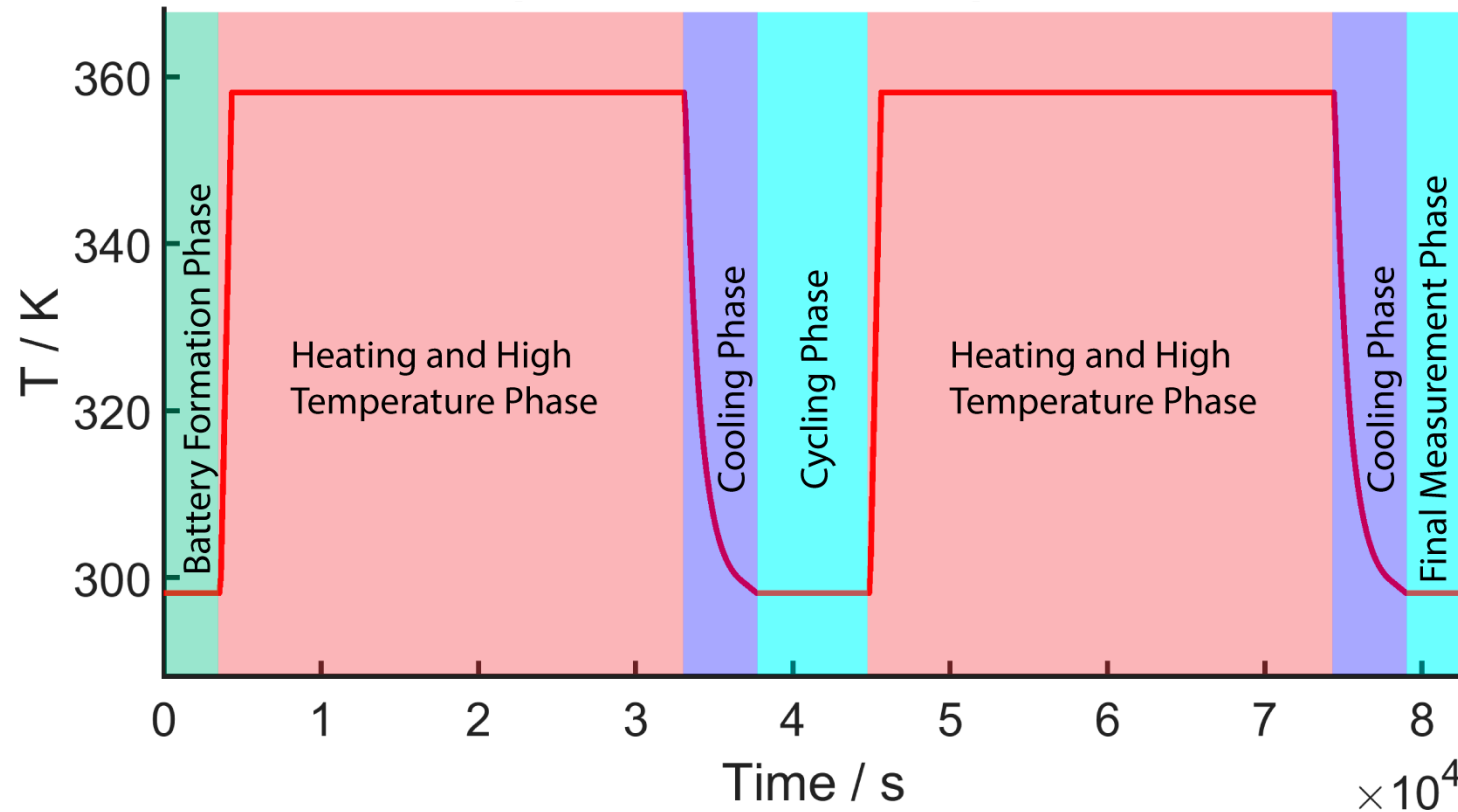
- Reactions and diffusion lead to changes in volume
- Volume change of VEs adapt dynamically

Implementation

$$x_{\text{dyn}}(t) = \frac{V_{\text{VE,dyn}}}{A_{\text{VE}}}$$

$$\frac{\partial c_a}{\partial t} = D_a \frac{\partial^2 c_a}{\partial x_{\text{dyn}}^2}$$

Experimental Procedure



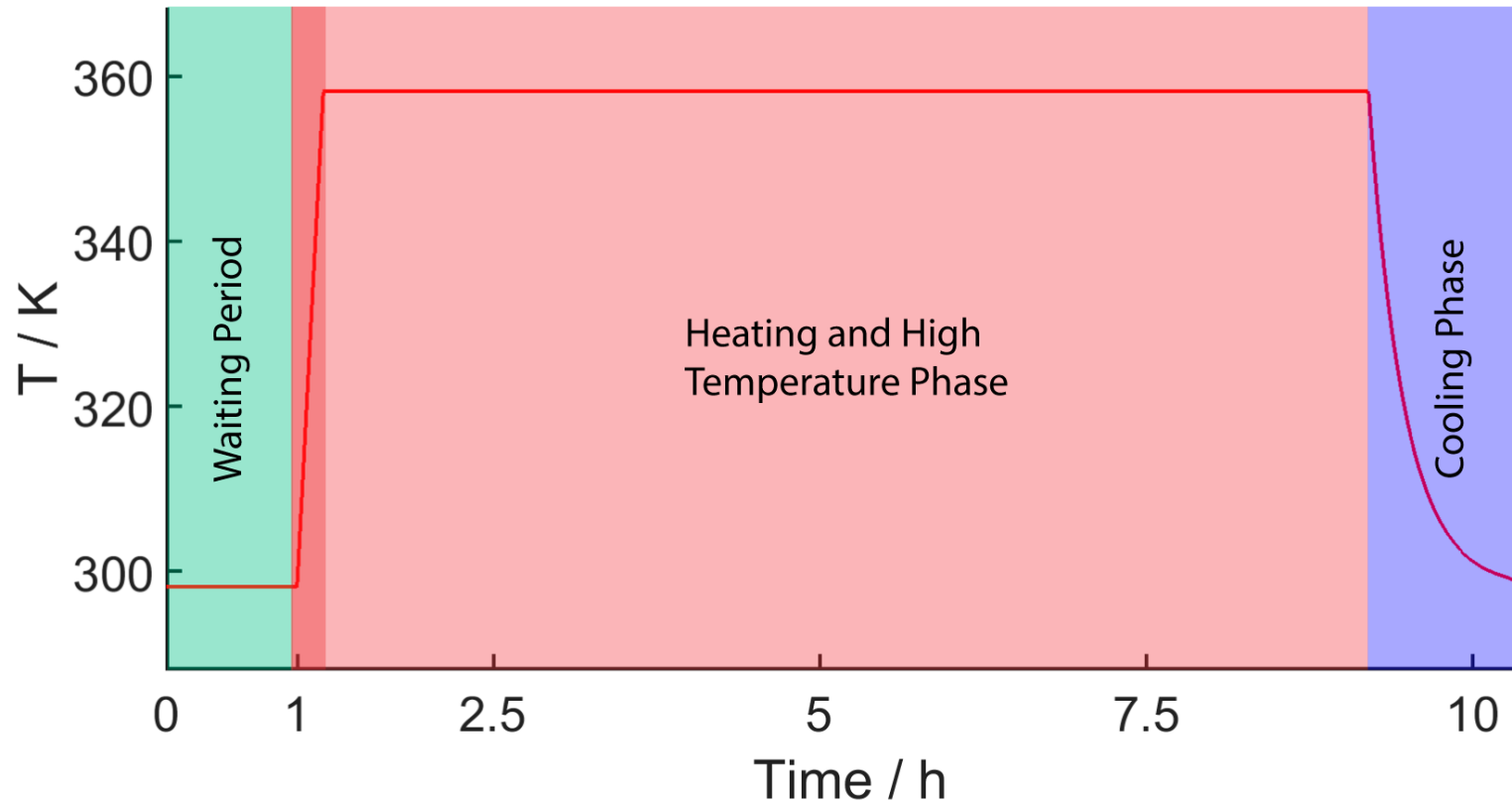
Procedure

- Battery formation
- Two heating periods w/ measurements
- Cycling phase
- Final measurement

Cell specification

- Lithium ion battery
- LiCoO_2 cathode
- Graphite anode

Simulation Procedure



Procedure 1 & 2

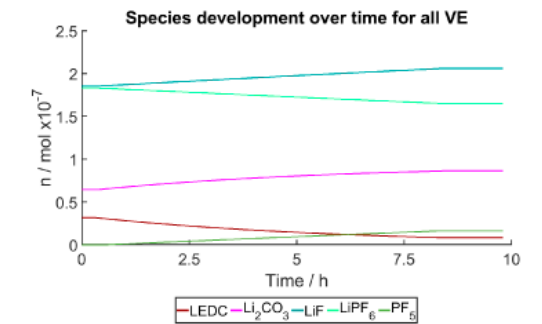
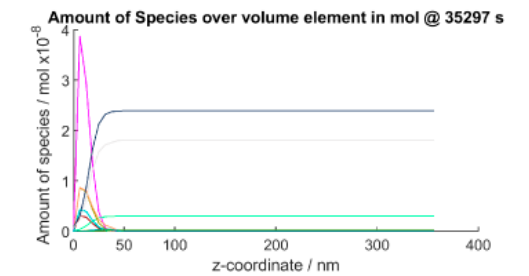
- $t = 4000 \text{ s}$ ($\sim 1.25 \text{ h}$)
- $T_0 = 25^\circ\text{C}$
- $T_{\max,1} = 25^\circ\text{C}$
- $T_{\max,2} = 85^\circ\text{C}$
- Heating rate = 0.083 K/s

Procedure 3

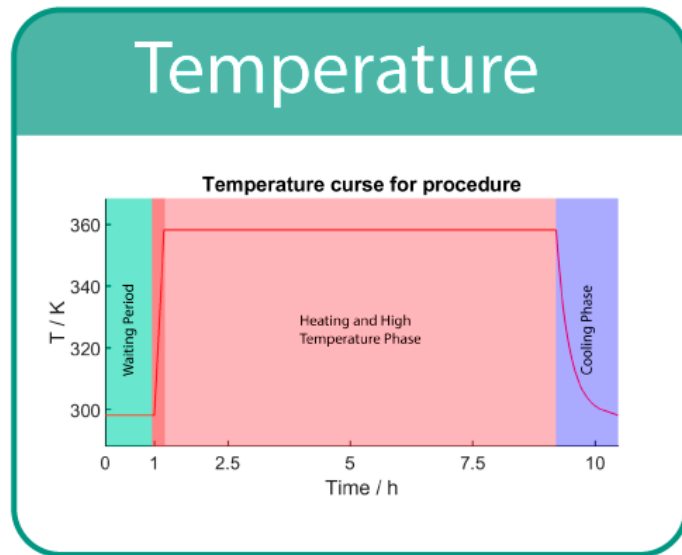
- $t = 37697 \text{ s}$ ($\sim 10.5 \text{ h}$)
- $T_0 = 25^\circ\text{C}$
- $T_{\max} = 85^\circ\text{C}$
- Heating rate = 0.083 K/s

Contents

Results and Evaluation

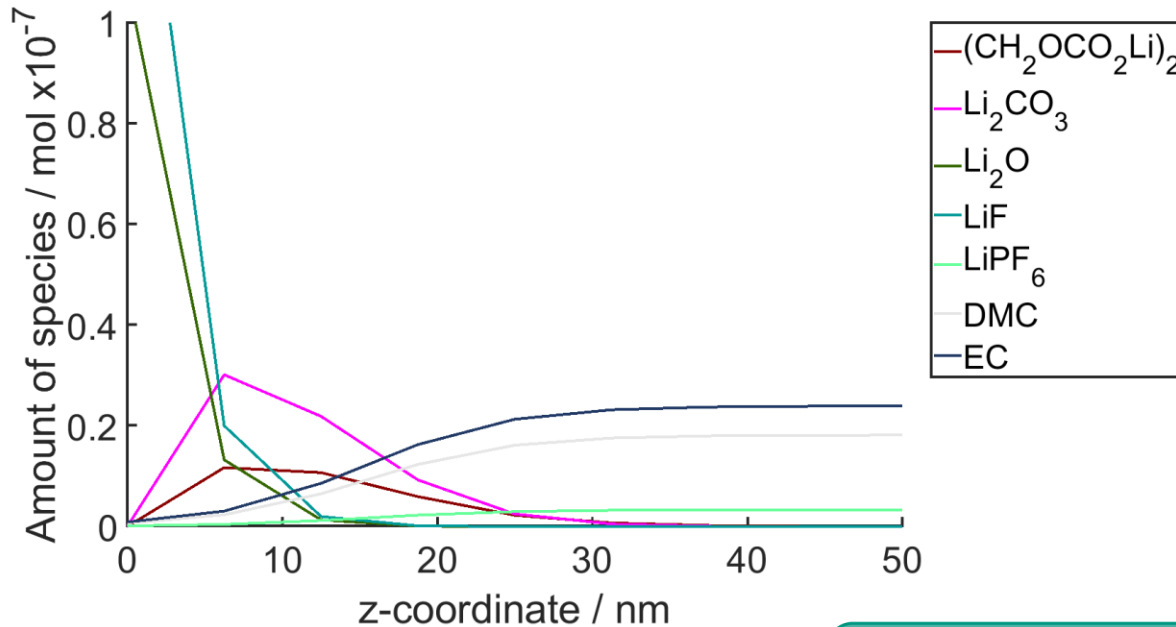


Evaluation and Results

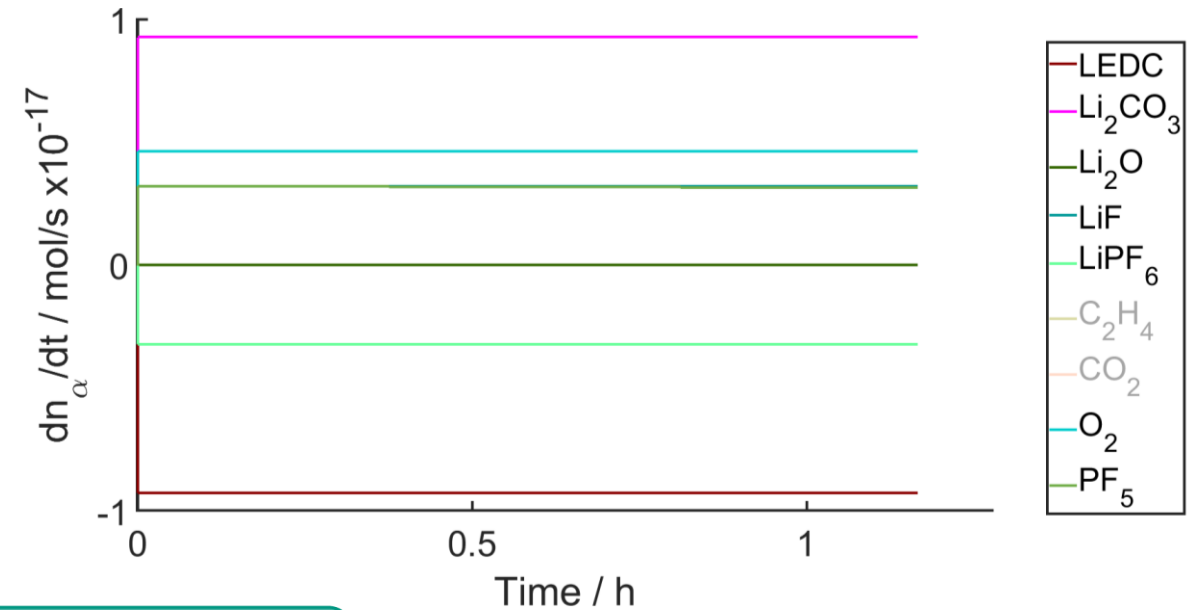


Temperature Dependency

End Amount of Species



Differential Amount of Species

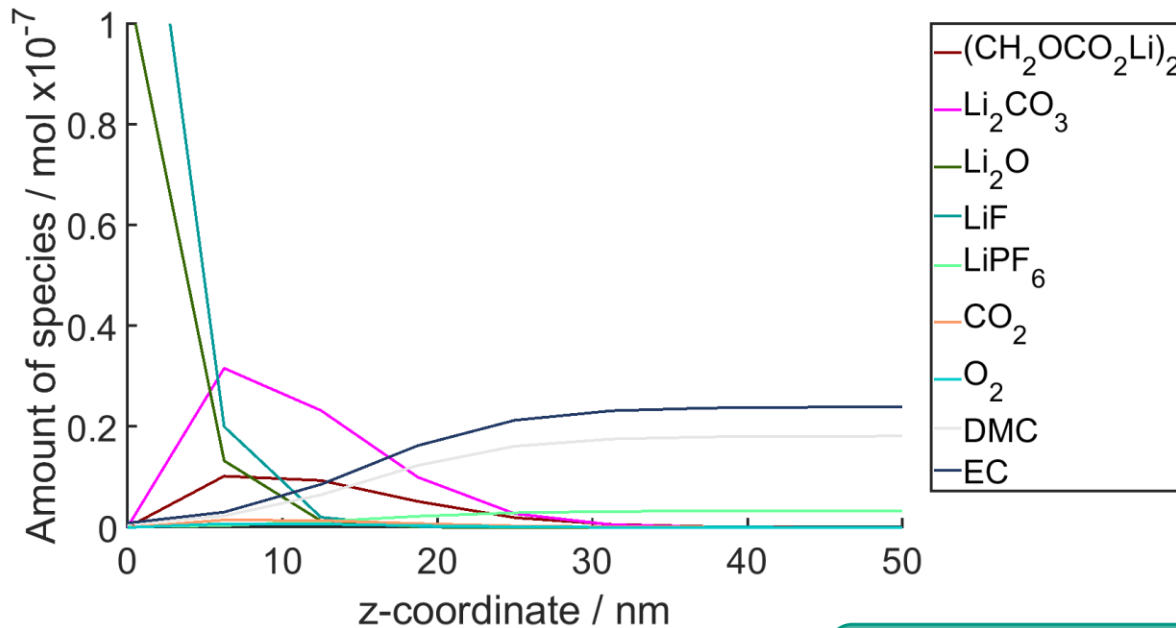


$T = 25^{\circ}\text{C}$ - Influence on reactions

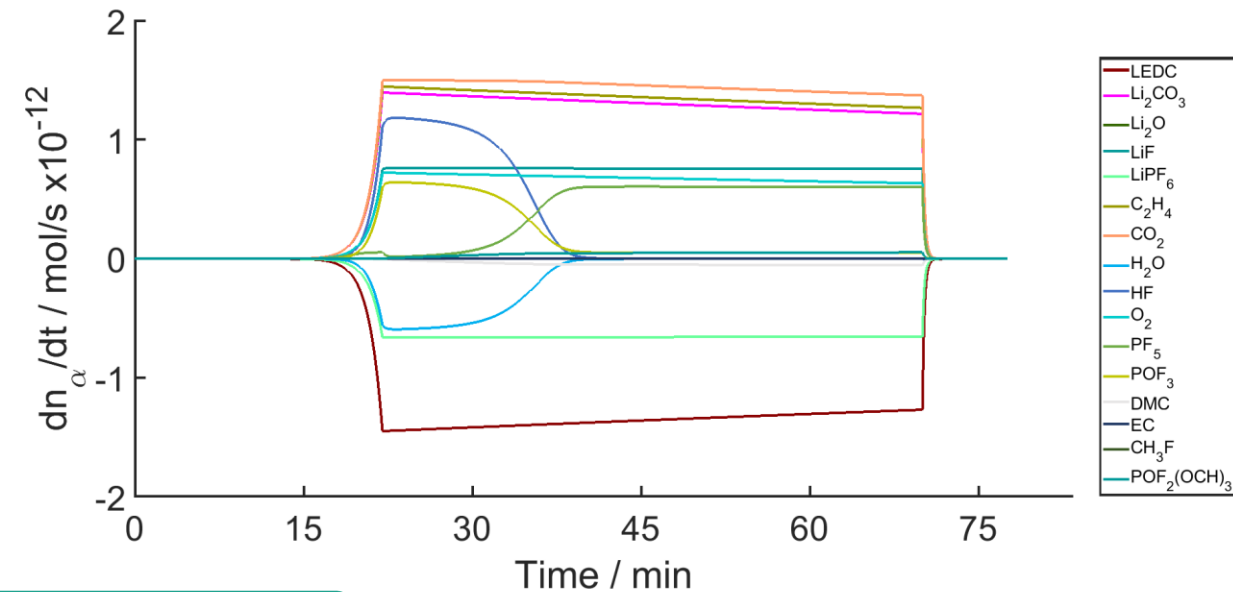
- Reaction rates low
- Differential changes at 10^{-17}

Temperature Dependency

End Amount of Species



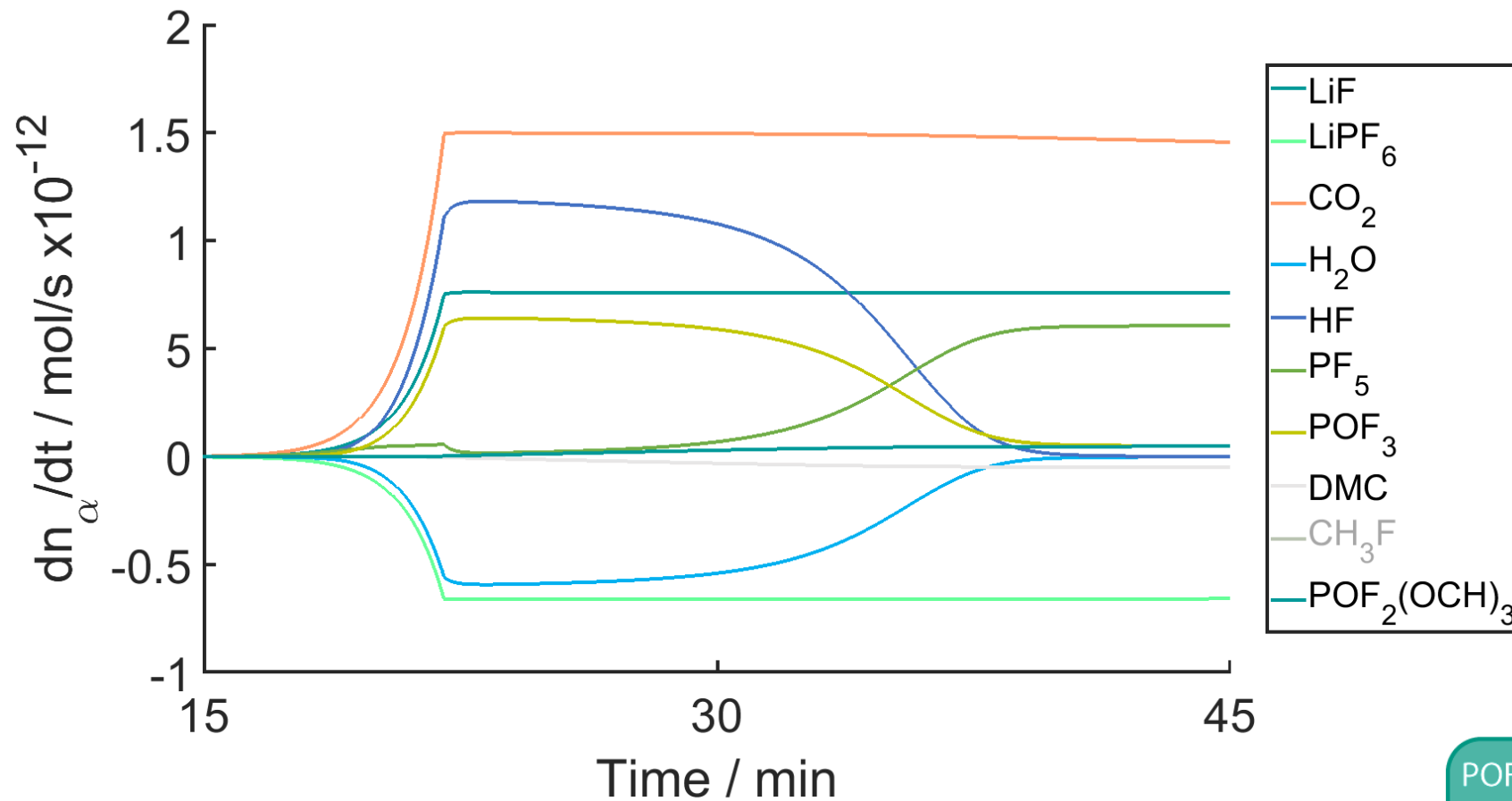
Differential Amount of Species



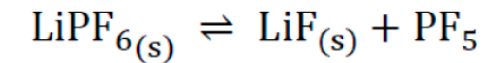
T = 85°C - Influence on reactions

- Reaction rates higher
- Differential changes at 10^{-12}

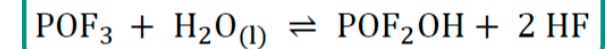
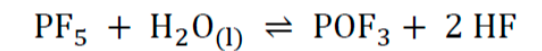
Temperature - Reactions



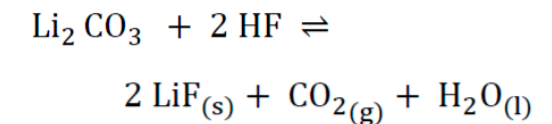
LiPF₆ Decomposition



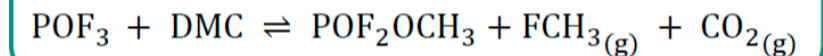
PF₅ / POF₃ Decomp. | HF Formation



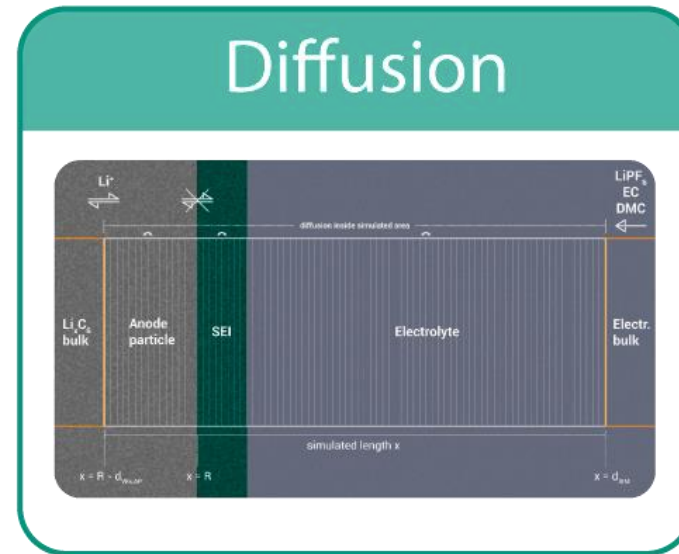
Li₂CO₃ Degradation with HF



POF₃ Degradation with DMC

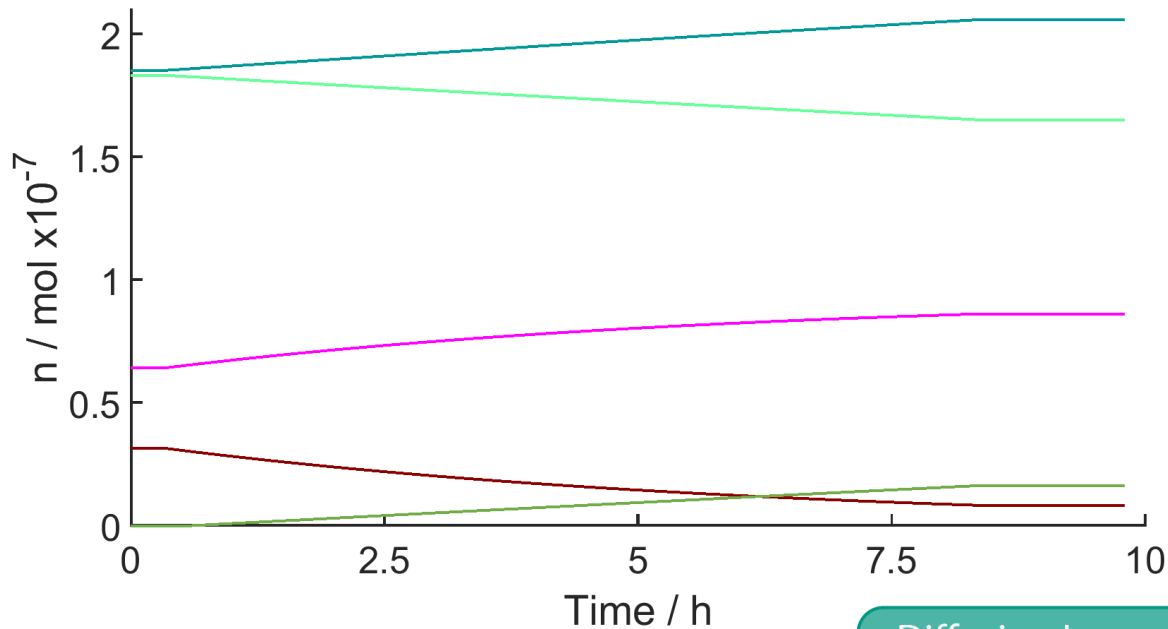


Evaluation and Results

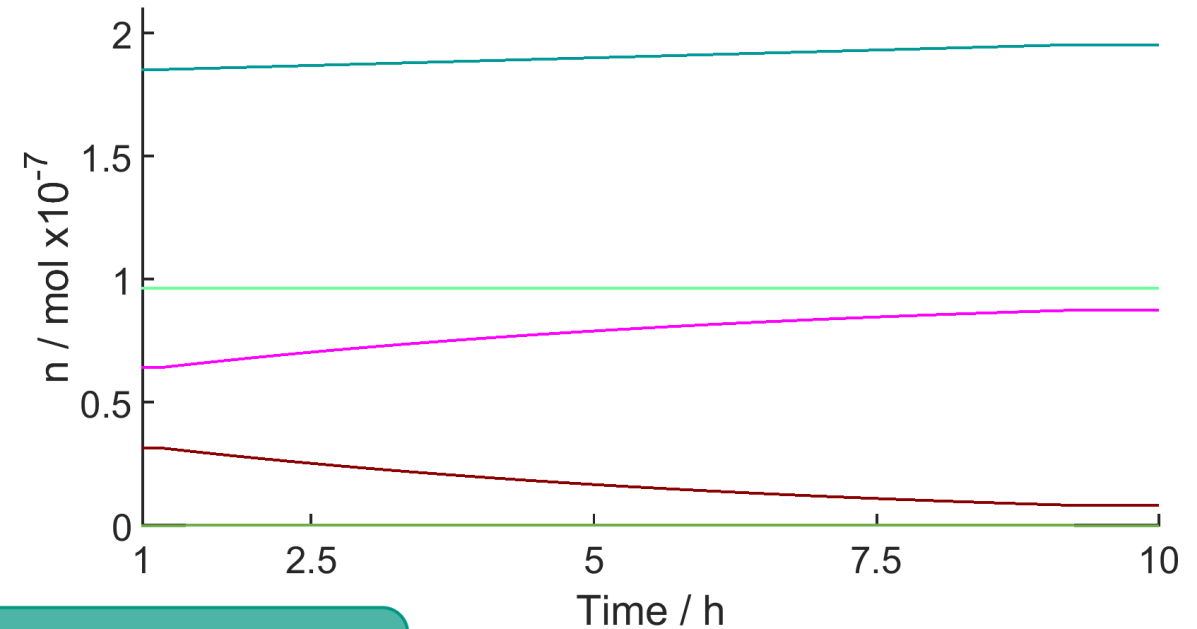


Diffusion – Impact on Simulation

Diffusion off

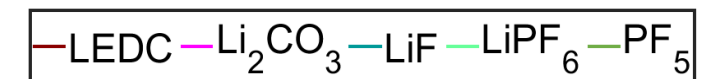


Diffusion on

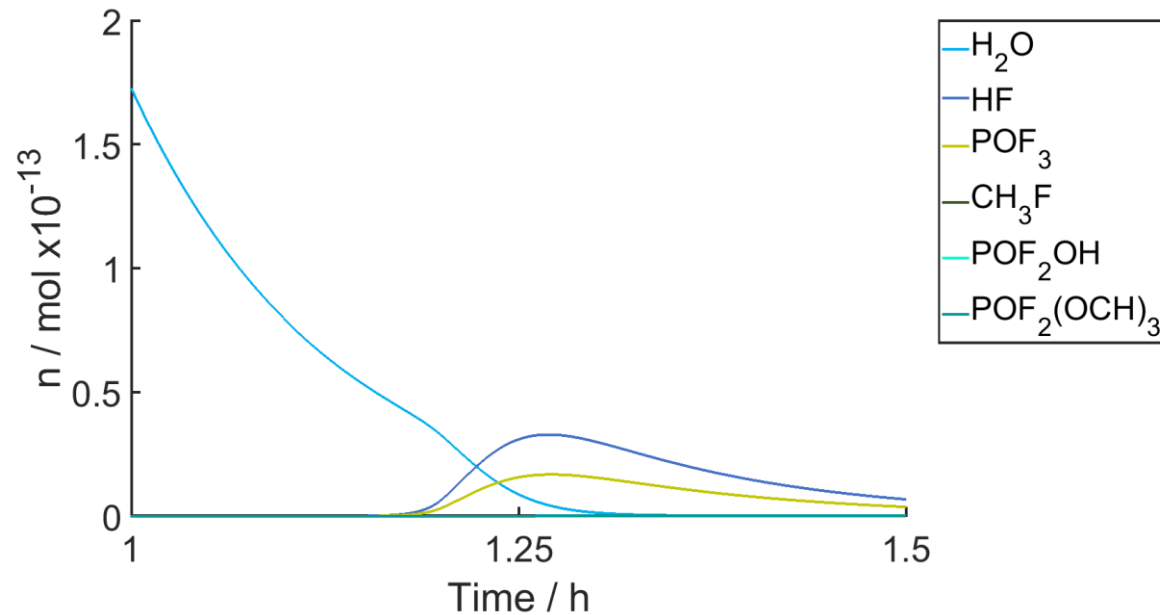


Diffusion Impact

- No impact on SEI species LEDC, Li_2CO_3 , LiF
- Major impact on electrolyte species

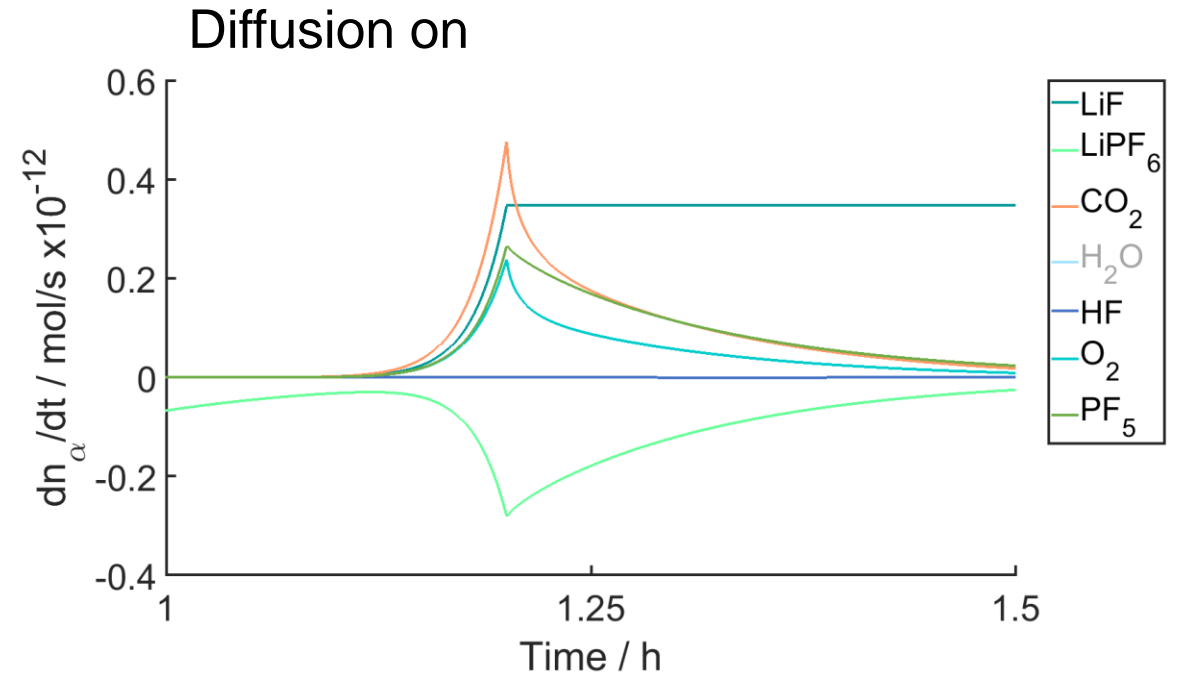


Diffusion – Heating Phase

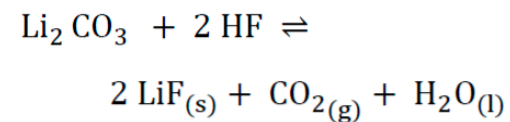


Diffusion Impact

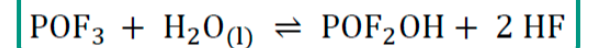
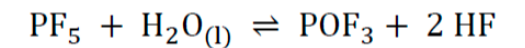
- Active decrease in electrolyte species concentration
- Shortage on water inhibits all further electrolyte reactions



Li_2CO_3 Degradation with HF

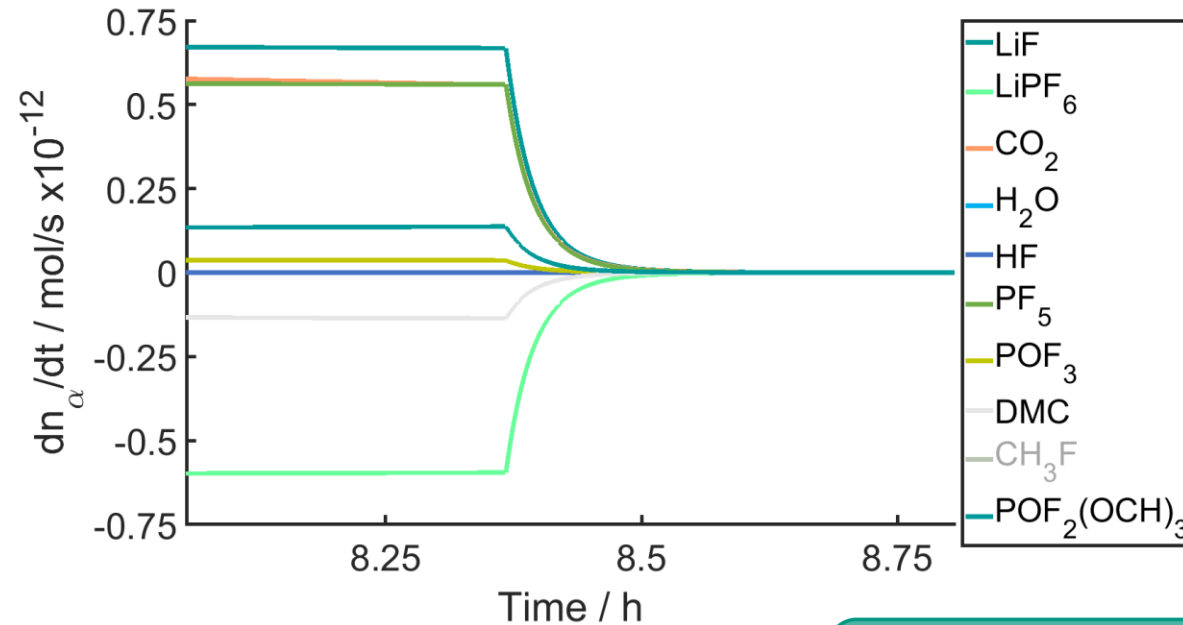


$\text{PF}_5 / \text{POF}_3$ Decomp. | HF Formation

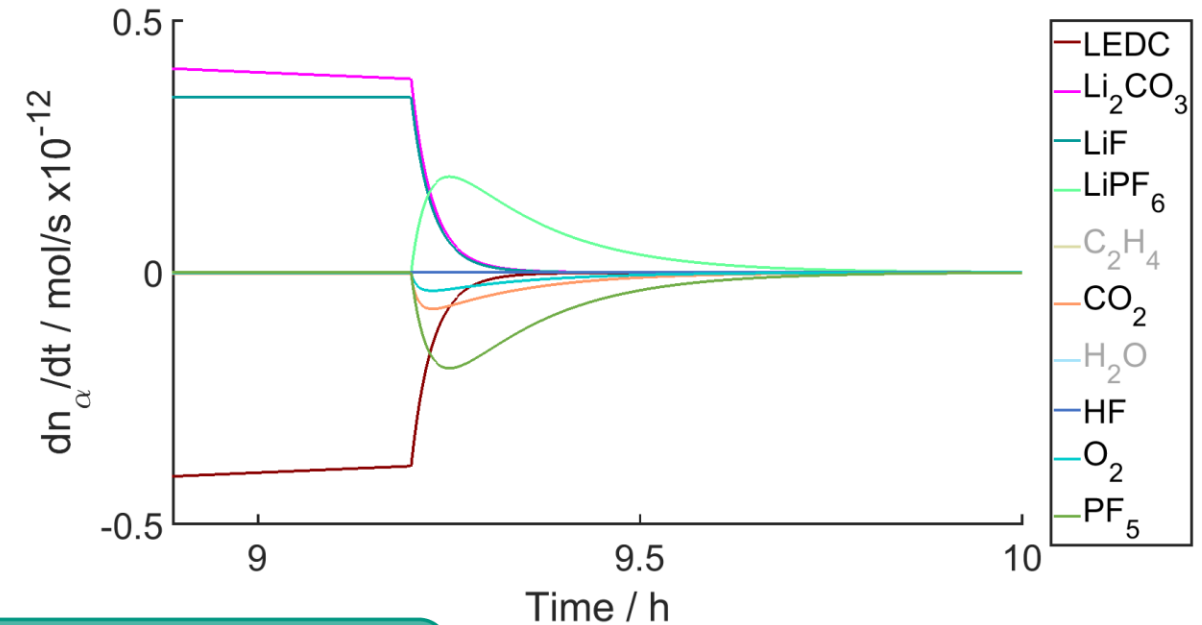


Diffusion – Cooling Phase

Diffusion off



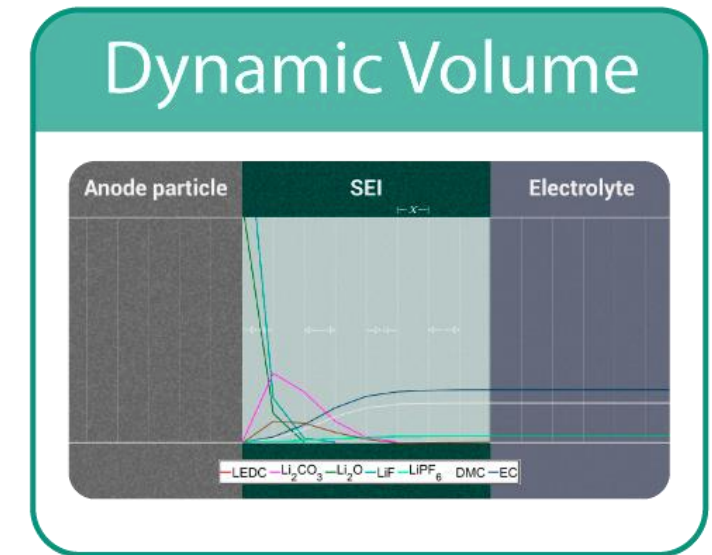
Diffusion on



Diffusion Impact

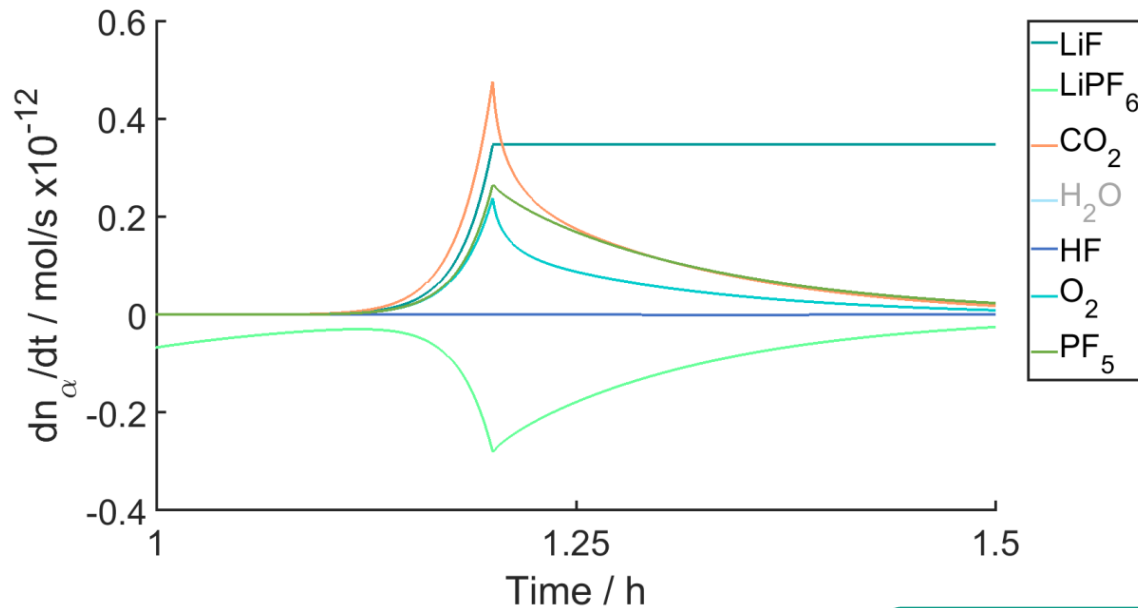
- Due to temperature drop, reactions are inhibited
- LiPF₆ from bulk flowing in
- Active decrease in concentration

Evaluation and Results

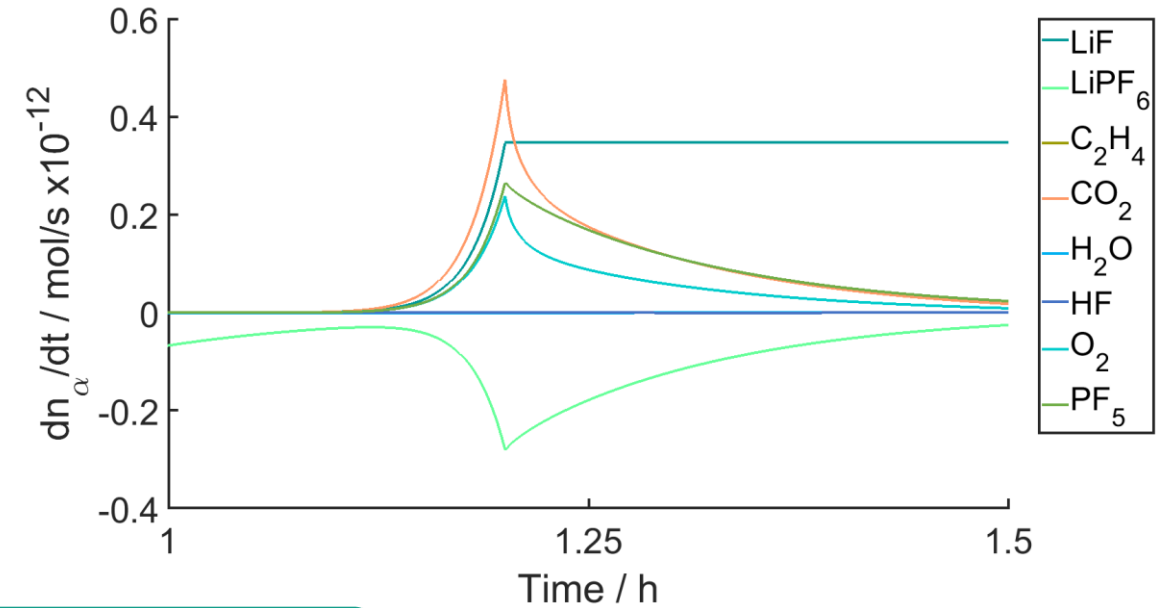


Dynamic Volume – Impact on Simulation

Static Volume



Dynamic Volume

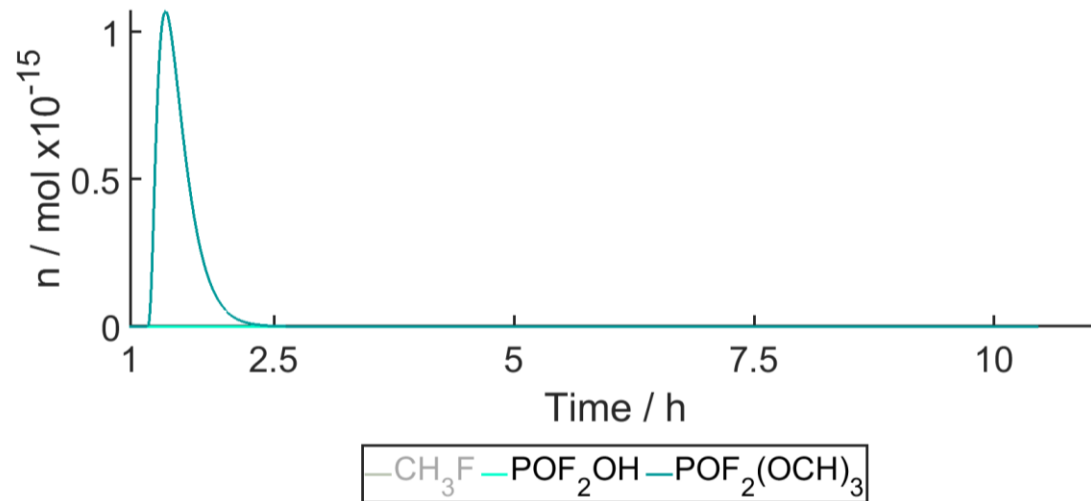


Dynamic Volume Impact

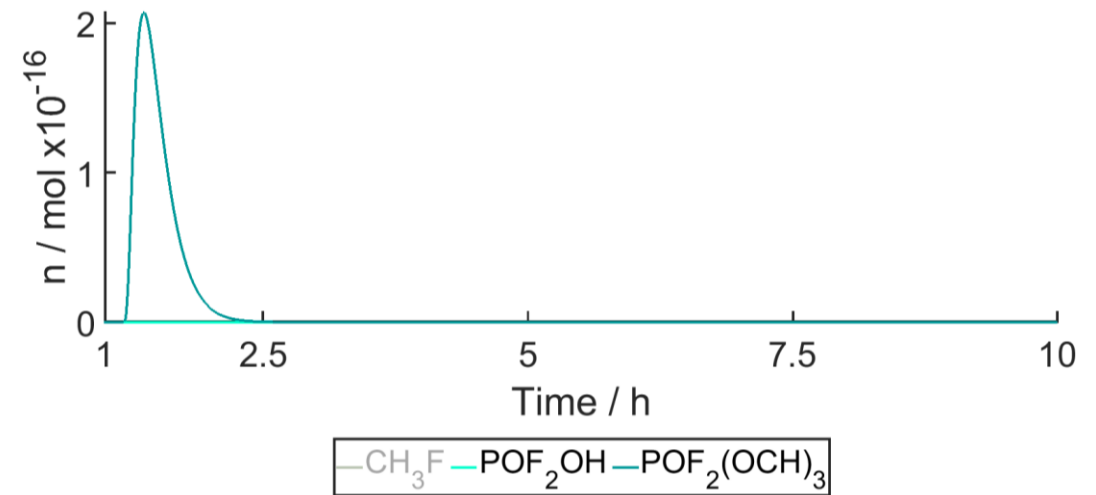
- No notable difference between static and dynamic volume

Dynamic Volume – Low Concentration Species

Static Volume



Dynamic Volume



Dynamic Volume Impact

- $\text{POF}_2(\text{OCH})_3$ amount differs in one order of magnitude
- Diffusion coefficient for dynamic volume one order of magnitude lower than for static

Improving the Model

- Finding the cause for decrease in concentration in diffusion model
- Adapting boundary conditions
- Finding workable diffusion coefficient ranges

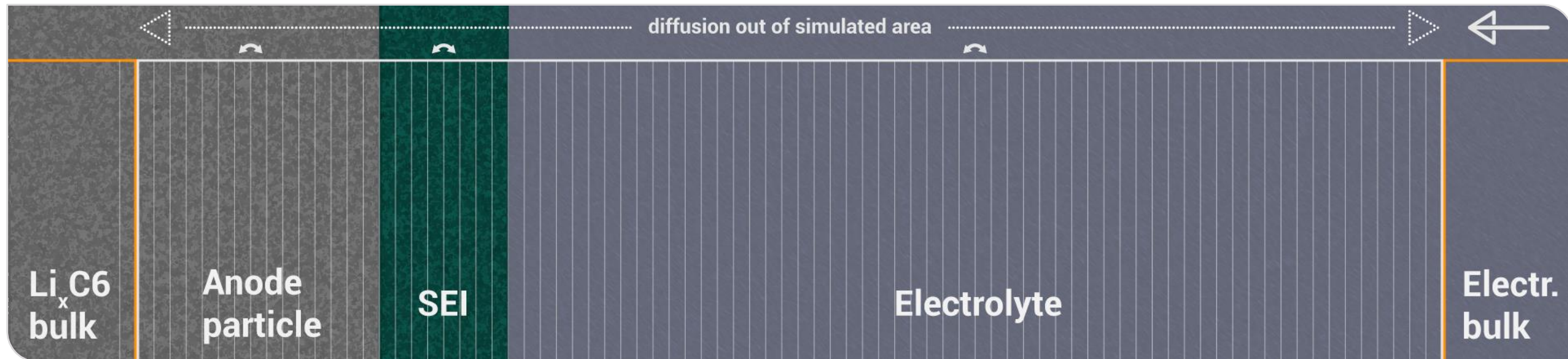
Further Implementations

- Implementing Lithium Diffusion between Anode and SEI
- Allowing for electrochemical reactions to take place
- Adding gas volumes to dynamic volume

Experimental Comparison

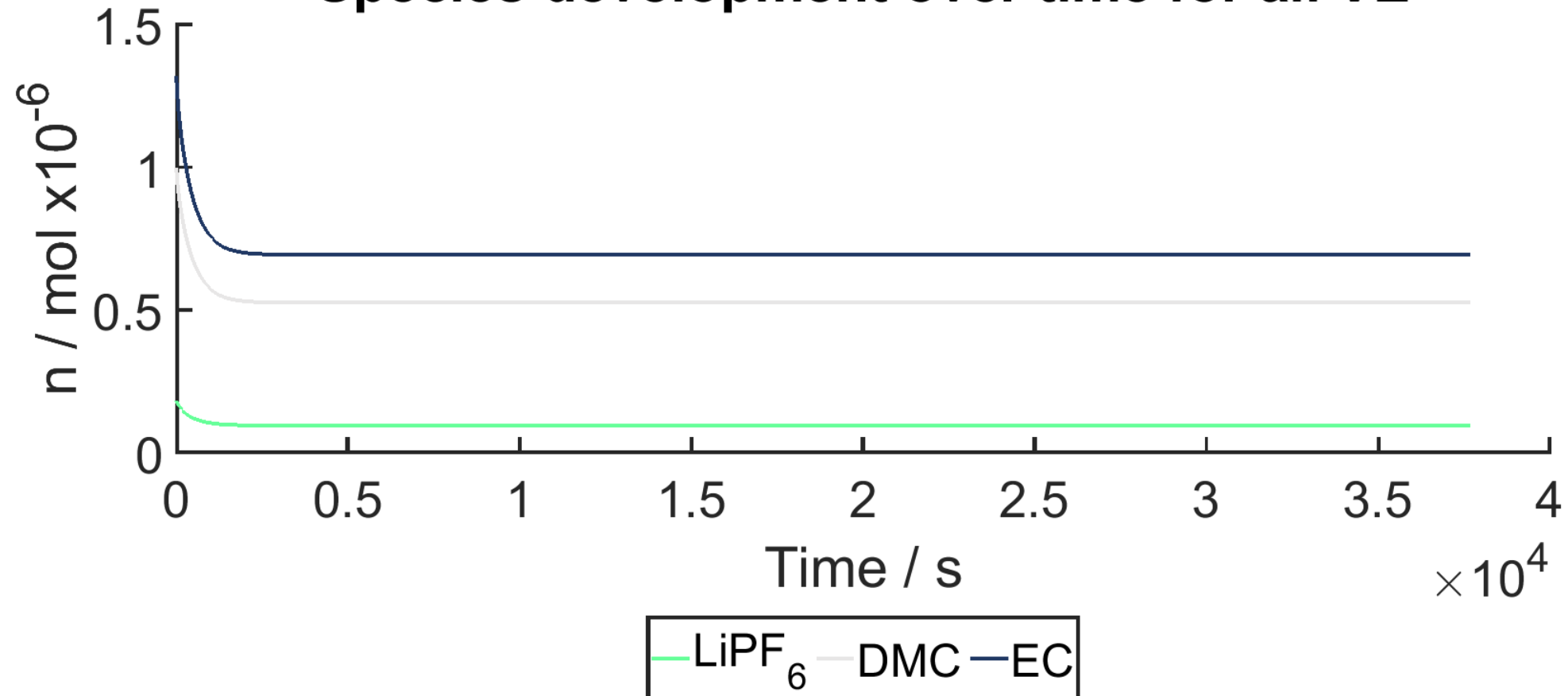
- Comparing experimental to simulated results
- Check for differences in electrolyte species

Thank you for your attention!

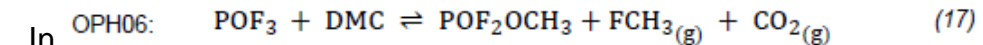
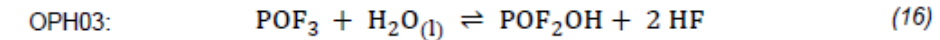
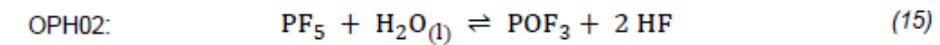
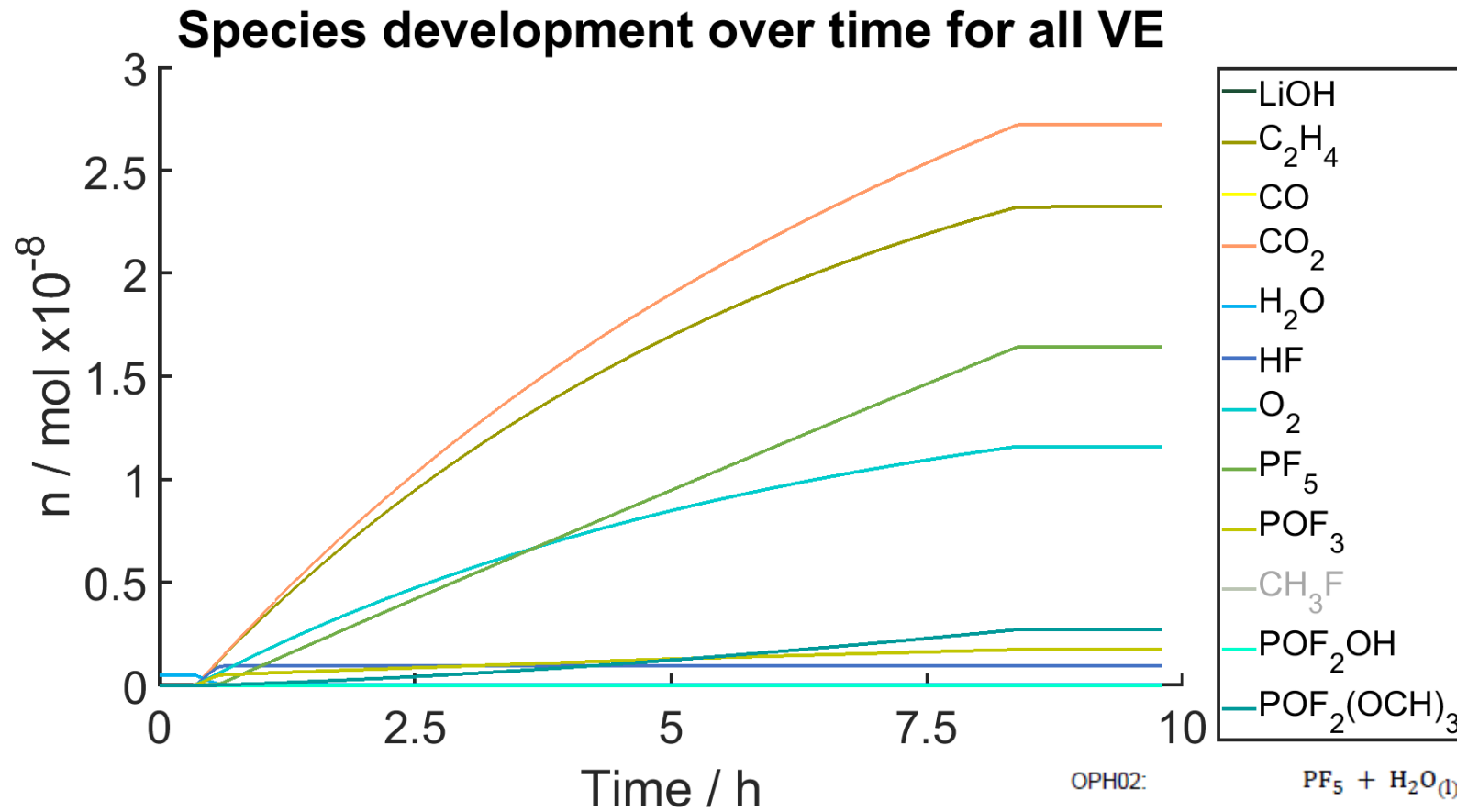


Diffusion – impact on simulation

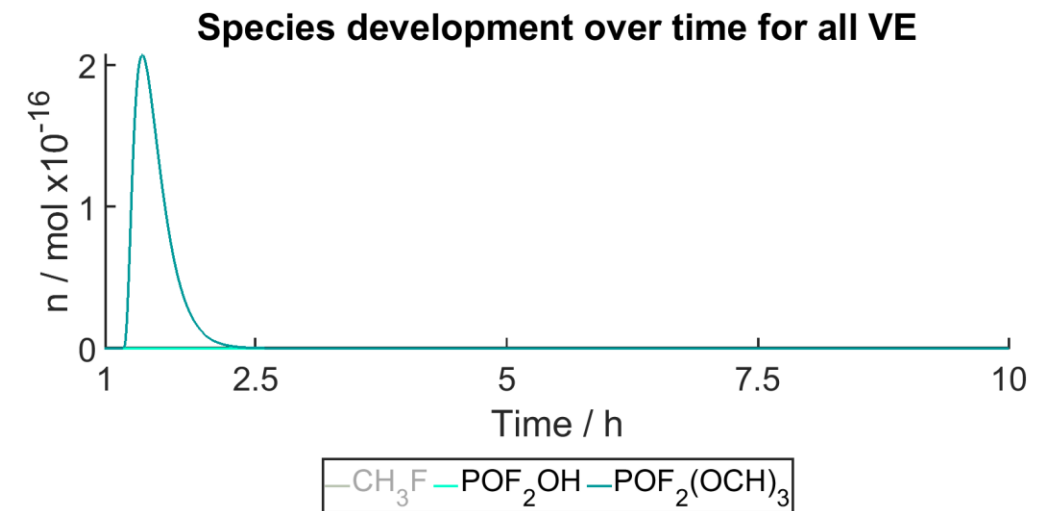
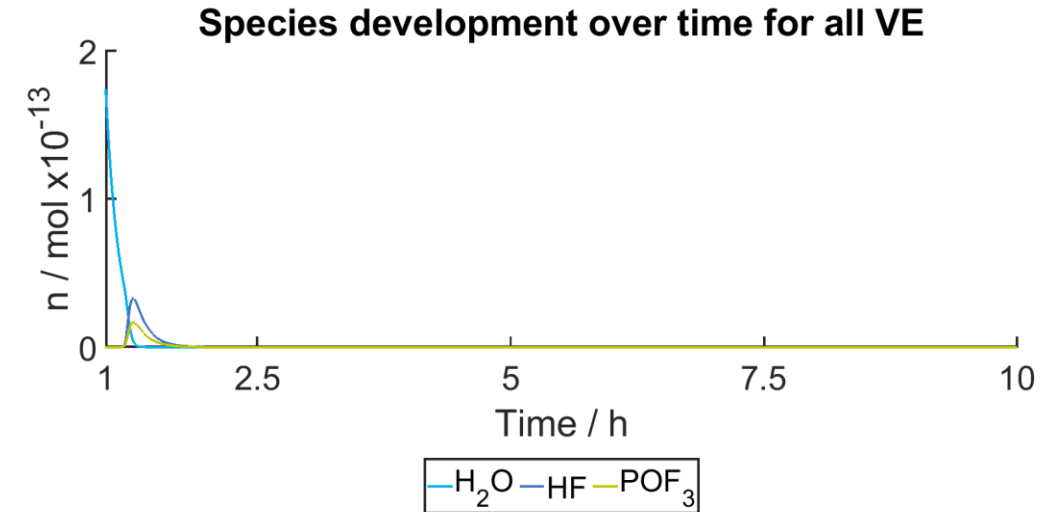
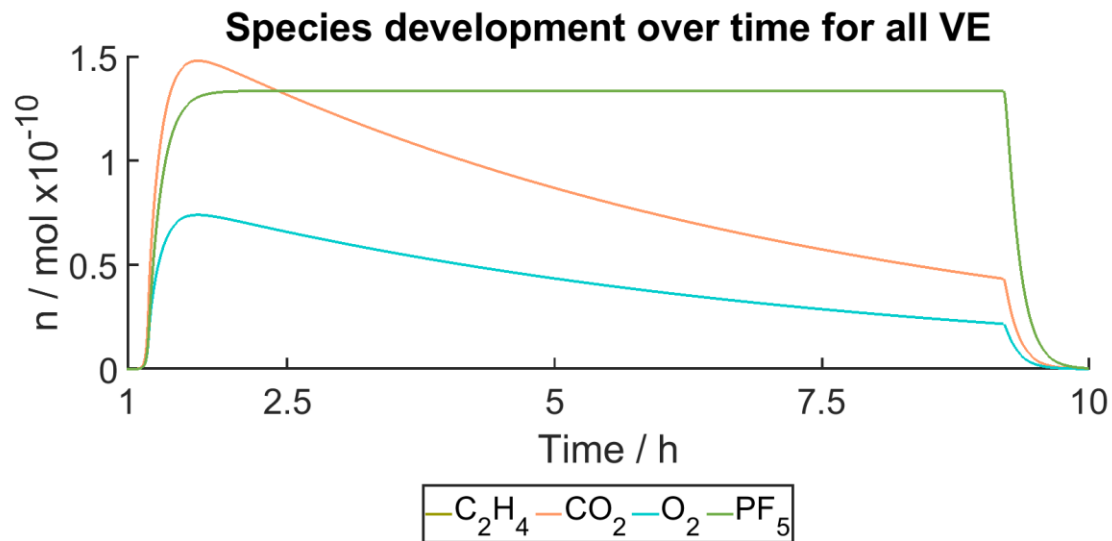
Species development over time for all VE



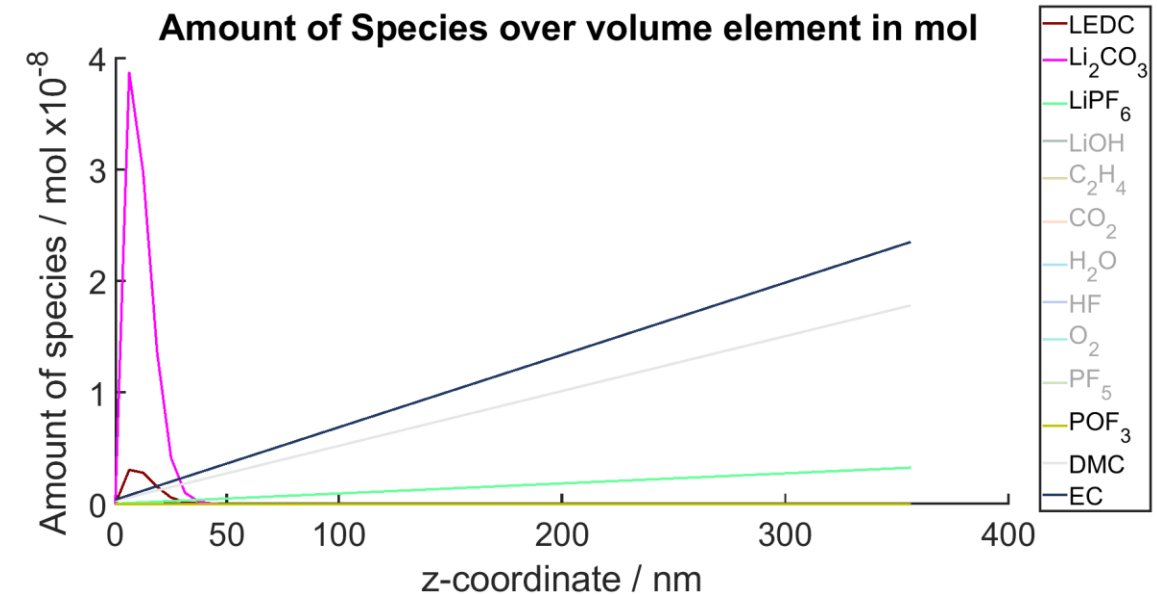
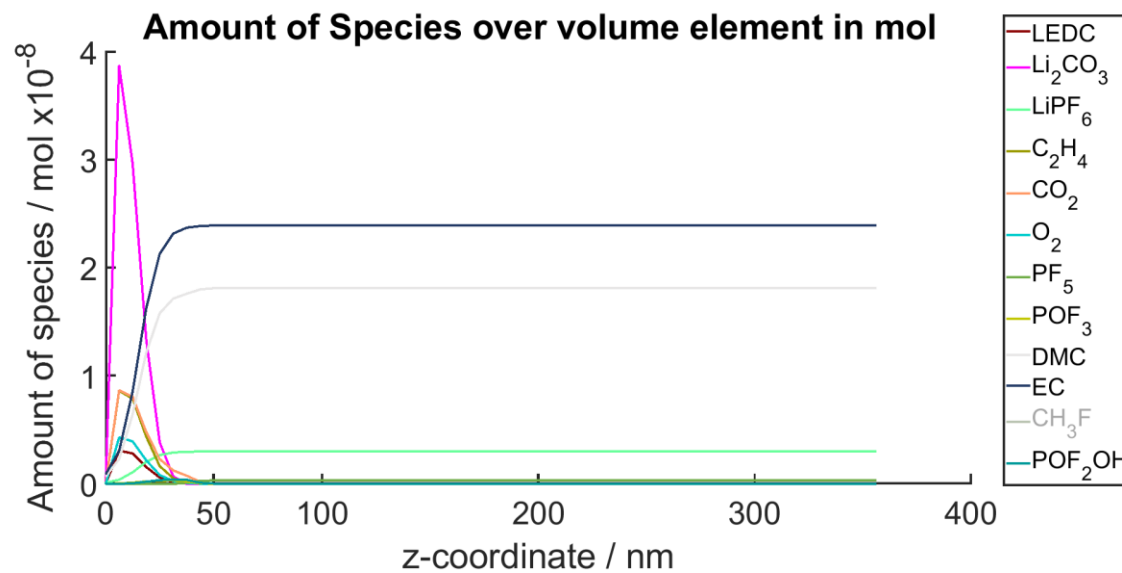
Diffusion – impact on simulation



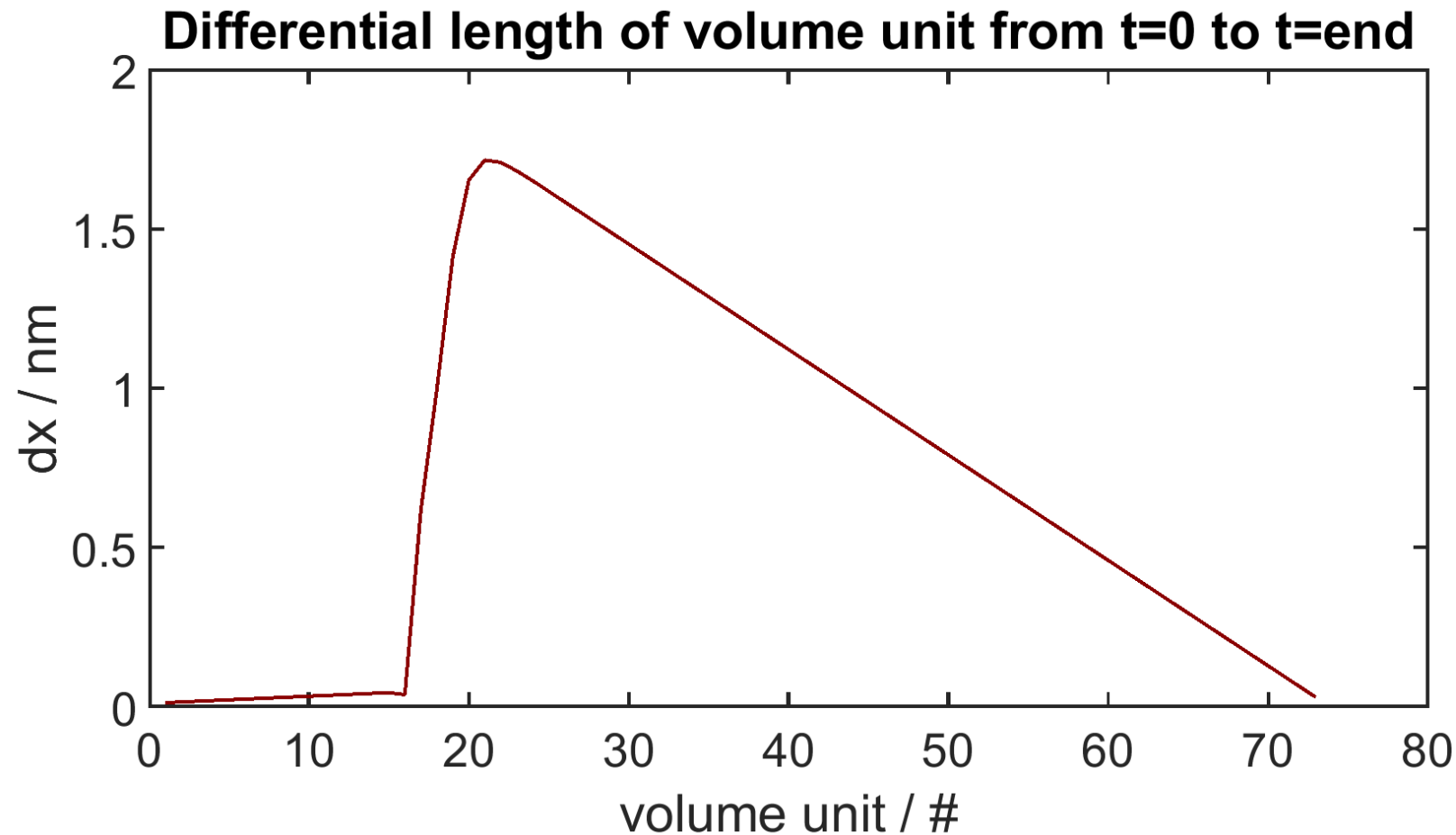
Diffusion – impact on simulation



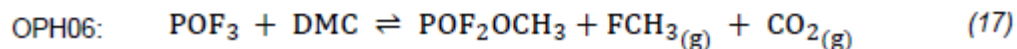
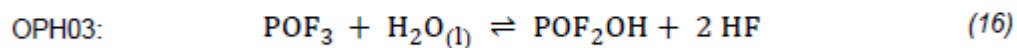
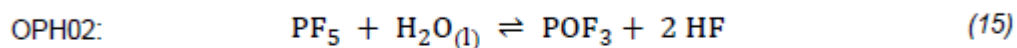
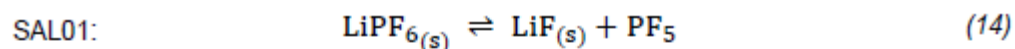
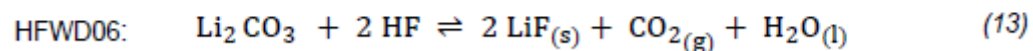
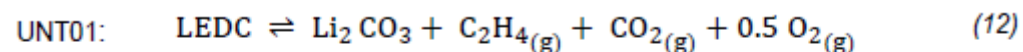
Diffusion – impact on simulation



Dynamic volume – impact on simulation



Reaction Parameters



Reaktionsbezeichnung	Aktivierungsenergie E_A [J/mol]	Geschwindigkeitskonstante k
EC01	$2 \cdot 10^5$	$1 \cdot 10^{13}$
EC02	$1,2 \cdot 10^5$	$1 \cdot 10^{13}$
EC03	$3 \cdot 10^5$	$1 \cdot 10^{13}$
DMC01	$1 \cdot 10^9$	0
DMC02	$1 \cdot 10^9$	0
IMP06	$2 \cdot 10^5$	$1 \cdot 10^{13}$
IMP07	$1 \cdot 10^6$	$1 \cdot 10^{13}$
IMP09	$2 \cdot 10^5$	$1 \cdot 10^{13}$
IMP10	$2 \cdot 10^5$	$1 \cdot 10^{13}$
UNT01	$1,77 \cdot 10^5$	$1 \cdot 10^{13}$
HFWD06	$1,1 \cdot 10^5$	$1 \cdot 10^{13}$
SAL01	$1,81 \cdot 10^5$	$1 \cdot 10^{13}$
OPH02	$1,38 \cdot 10^5$	$1 \cdot 10^{13}$
OPH03	$2 \cdot 10^5$	$1 \cdot 10^{13}$
OPH06	$1,8 \cdot 10^5$	$1 \cdot 10^{13}$

WS R3DT GmbH | Aufgaben

Aufgabengebiete

- Technische Dokumentation der Software
- Aufbau einer Knowledge Base für Entwicklung und Kunden
- Qualitätssicherung
- Kundenbetreuung
 - technischer Support
 - Installation
 - Softwarepräsentation
- Konzeptionelle und operative Begleitung neuer Softwarefeatures und -releases

Aufgabengebiet

- Dokumentation
- Aufbau Testszenarien/-prozesse
- Strukturierung QA
- Meetings mit Kunden (digital und vor Ort)
- Erstellung Graphiken, Webdesign
- Erstellung Videoinhalte
- Mitarbeit Cloud Security Prüfungen
- Konzept und Vermittlung Feature Integration

WS R3DT GmbH | Knowledge Base

[Knowledge Base](#)[FAQ](#)[Support anfordern](#)[EN](#)[→ Log in](#)

Sie schaffen das, wir helfen Ihnen!



Quick Guide

Der schnellste Weg zu XR-EASY.

[Zum Quick Guide](#)

Handbuch

Dieses Handbuch hilft beim Einrichten und Kennenlernen der VR-Software XR-EASY®.

[Zum Handbuch](#)

FAQ

Häufig gestellte Fragen von Produktinformationen, über Bedienung bis zur Fehlerbehebung.

[Zur FAQ](#)

Support

Schreiben Sie uns eine E-Mail. Wir helfen Ihnen!

[Zum Support](#)

Cloud Support

Alles über die Einrichtung der XR-EASY Cloud durch IT-Personal.

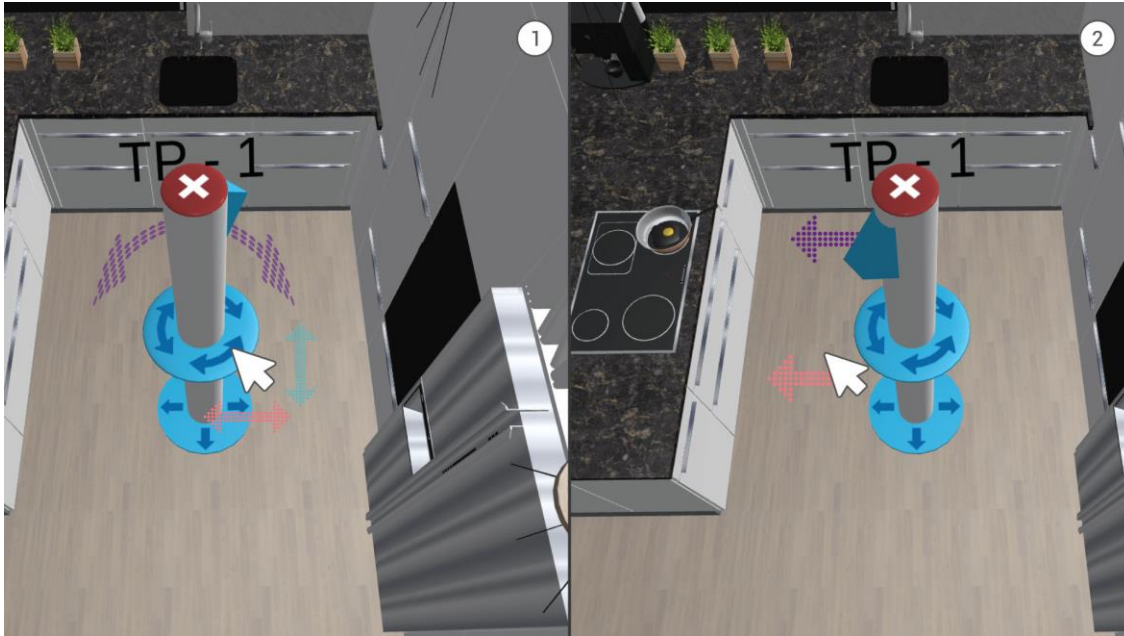
[Zum IT Support](#)

WS R3DT GmbH | Konzepte

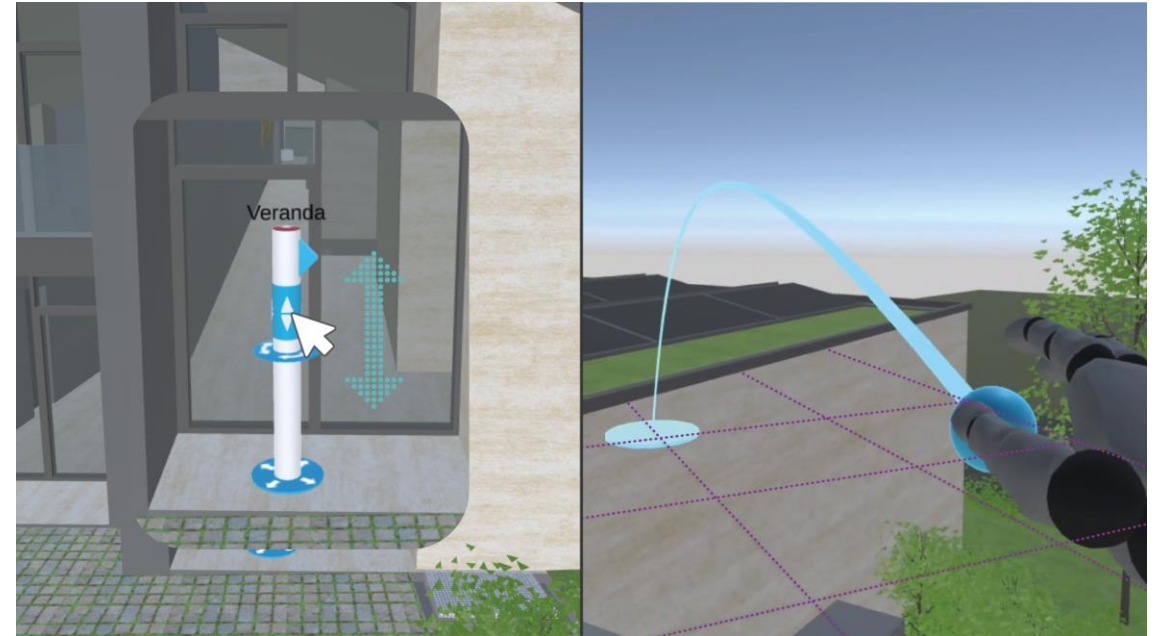
Hand Menu variants	
<ul style="list-style-type: none">VARIANTMENUSBUTTONSCODE - B -Button, M -Menu	
Variant	Functions
M1 /// SA HOST NO WORK	MOVEALL B57 TELEPORT M3 0 SESSION M11
M2 /// PC VR NO WORK HOST	TELEPORT M3 0 GENERAL TOOLS M4 SESSION M11
M3 /// SA NO WORK HOST	MOVEALL B57 TELEPORT M3 0 MEASUREMENT B20 SESSION M11
M4 /// SA PC VR WORK PERM HOST JOIN	WORKVR B49 TELEPORT M3 0 SESSION M11
M5 /// PC VR WORK ON HOST JOIN	TELEPORT M3 1 OBJECT TOOLS M5 GENERAL TOOLS M4 MODULES M6 SESSION M11
M6 /// SA WORK ON HOST JOIN	TELEPORT M3 1 OBJECT TOOLS M5 MEASUREMENT B20 MODULES M6 SESSION M11
M7 /// SA JOIN NO WORK	TELEPORT M3 0 SESSION M11

Permission Level VR - Menus						
	Free			Licensed		
	PC VR	StandAlone (SA)	StandAlone Studio	PC VR - Pro	PC VR - Studio	PC VR - Showroom
Offline	M2 /// PC VR NO WORK HOST	M3 /// SA NO WORK HOST	M3 /// SA NO WORK HOST	M5 /// PC VR WORK ON HOST	M3 /// SA NO WORK HOST	M6 /// SA WORK ON HOST
	TELEPORT M3 0 GENERAL TOOLS M4 SESSION M11	MOVEALL B57 TELEPORT M3 0 MEASUREMENT B20 SESSION M11	MOVEALL B57 TELEPORT M3 0 MEASUREMENT B20 SESSION M11	TELEPORT M3 1 OBJECT TOOLS M5 GENERAL TOOLS M4 MODULES M6 SESSION M11	MOVEALL B57 TELEPORT M3 0 MEASUREMENT B20 SESSION M11	TELEPORT M3 1 OBJECT TOOLS M5 MEASUREMENT B20 MODULES M6 SESSION M11
COOP-Host: Work	M2 /// PC VR NO WORK HOST	M3 /// SA NO WORK HOST	M3 /// SA NO WORK HOST	M5 /// PC VR WORK ON HOST	M1 /// SA NO WORK HOST	M6 /// SA WORK ON HOST
	TELEPORT M3 0 GENERAL TOOLS M4 SESSION M11	MOVEALL B57 TELEPORT M3 0 MEASUREMENT B20 SESSION M11 Notes: • If you host as SA user, you cannot give permission	MOVEALL B57 TELEPORT M3 0 MEASUREMENT B20 SESSION M11 Notes: • If you host as SA user, you cannot give permission	TELEPORT M3 1 OBJECT TOOLS M5 GENERAL TOOLS M4 MODULES M6 SESSION M11	MOVEALL B57 TELEPORT M3 0 SESSION M11	TELEPORT M3 1 OBJECT TOOLS M5 MEASUREMENT B20 MODULES M6 SESSION M11
COOP-Host: Viewer	M2 /// PC VR NO WORK HOST	M3 /// SA NO WORK HOST		M4 /// PC VR WORK PERM HOST	M1 /// SA NO WORK HOST	M4 /// SA WORK PERM HOST
	TELEPORT M3 0 GENERAL TOOLS M4 SESSION M11 Notes: - If you host as license free user, you cannot give nor take permission			WORKVR B49 TELEPORT M3 0 SESSION M11		WORKVR B49 TELEPORT M3 0 SESSION M11
COOP-Join: Work	M5 /// PC VR WORK ON JOIN	M6 /// SA WORK ON JOIN		M5 /// PC VR WORK ON JOIN	M1 /// SA NO WORK JOIN	M6 /// SA WORK ON JOIN
	TELEPORT M3 1 OBJECT TOOLS M5 GENERAL TOOLS M4	TELEPORT M3 1 OBJECT TOOLS M5 MEASUREMENT B20		TELEPORT M3 1 OBJECT TOOLS M5 GENERAL TOOLS M4		TELEPORT M3 1 OBJECT TOOLS M5 MEASUREMENT B20

WS R3DT GmbH | Graphik



Darstellung: Bewegungsmöglichkeiten eines Elements



Darstellung: Extra-Funktionalität mit perspektivischem Raster